Semiclassical Dynamics of Loop Quantum Gravity

Der Naturwissenschaftlichen Fakultät

der Friedrich-Alexander-Universität
Erlangen-Nürnberg
zur
Erlangung des Doktorgrades Dr. rer. nat.
vorgelegt von

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Als Dissertation genehmigt von der Naturwissenschaftlichen Fakultät
der Friedrich-Alexander-Universität Erlangen-Nürnberg

Tag der mündlichen Prüfung: 18.01.2022

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Acknowledgements

At first I would like to express my gratitude to my supervisor Prof. Dr. Kristina Giesel for her insightful comments and suggestions as well as her patience during my phd study. I am deeply grateful to Director of Research Dr. Simone Speziale to examine my work as a referee. Moreover, I would like to thank Prof. Dr. Michael Schmiedeberg and Prof. Dr. Uli Katz to be willing to support my defense. Finally, I owe special thanks to the Heinrich-Böll-Stiftung for the scholarship that allowed me to conduct this thesis.

Contents

Zusammenfassung

Semiklassische Dynamik der Schleifenquantengravitation

Das Thema dieser Arbeit ist die Untersuchung und Verbesserung der semiklassischen Techniken innerhalb der Schleifenquantengravitation (SQG) mit dem Ziel zu überprüfen, ob die betrachteten quantisierten Größen die entsprechenden klassischen Größen korrekt widerspiegeln. Überlegungen und Arbeiten im Rahmen der semiklassischen Störungstheorie unter Verwendung von sogenannten Komplexifizierer-Kohärenten-Zuständen dazu gibt es bereits in [2, 3, 4, 5]. Die neuen Aspekte dieser Arbeit liegen zum einen darin, dass eine andere Klasse von Operatoren, die als physikalische Hamiltonoperatoren bezeichnet werden, unter semiklassischen Gesichtspunkten untersucht wird und zum anderen eine Vielzahl von Techniken über die semiklassische Störungstheorie hinaus betrachtet wird. Physikalische Hamiltonfunktionen können im Kontext der Allgemeinen Relativitätstheorie (ART) u.a. aus der Addition zusätzlicher Materiewirkungen zur Gravitationswirkung, der Einstein-Hilbert-Wirkung, resultieren. Die sich daraus ergebende physikalische Hamiltonfunktion wird dann für gewöhnlich mit Hilfe der sogenannten reduzierten Phasenraumquantisierung quantisiert, was auf den physikalischen Hamiltonoperator führt. Im Rahmen dieser Arbeit zeigte sich, dass abhängig von der Art der gekoppelten Felder Modelle, die Dirac quantisierbar sind, siehe Teil II, nicht notwendigerweise auch mit Hilfe der Methode der reduzierte Phasenraumquantisierung, siehe Teil III, quantisiert werden können. Je nach funktionaler Form des physikalischen Hamiltonoperators kann die Übertragbarkeit der semiklassischen Techniken aus [4] auf physikalische Hamiltonoperatoren technisch sehr aufwendig sein und erfordert eine genauere Analyse des Problems als bisher in der Literatur erfolgt ist. Daher wird im Rahmen dieser Arbeit versucht, neue semiklassische und alternative Techniken, insbesondere semiklassische Zustände, welche die funktionale Form der physikalischen Hamiltonoperatoren berücksichtigen, zu finden bzw. zu entwickeln.

Teil I legt die Motivation für die Arbeit dar und erläutert ihren Aufbau.

Im Teil II der Arbeit wird die Entwicklung von der ART zur Formulierung der SQG beschrieben [6, 7, 8, 9, 10, 11, 12, 13]. Dabei wird in Abschnitt 1 ausgehend von den Einsteingleichungen zunächst gezeigt, dass diese sich aus der Variation der Einstein-Hilbert-Wirkung ergeben. Die Einstein-Hilbert-Wirkung enthält die Lagrangefunktion der ART mit der nachfolgend weitergearbeitet wird. Nach der Einführung der ADM-Zerlegung [14], welche anschaulich der Zerlegung in Zeit- und Raumanteile entspricht, wird die Legendretransformation vom Lagrange- zum Hamiltonformalismus für die ART ausgeführt. Ein wichtiges Resultat ist, dass die Hamiltonfunktion für die ART nur aus der Summe von Zwangsbedingungen besteht, welche zeitliche und räumliche Diffeomorphismen als Eichtransformationen der ART erzeugen. Es folgt die Bestimmung der Zwangsbedingungsalgebra, welche als Hyperflächendeformations-Algebra [15] oder auch Dirac-Algebra [16] bezeichnet wird, sowie eine Diskussion ihrer Bedeutung. Am Ende des Abschnitts 1 erfolgt der Übergang von den Orts- und Impuls-Phasenraumvariablen zu den neuen Ashtekar-Variablen, welche die Grundlage der Quantisierung bilden. Hier setzt Abschnitt 2 über den Übergang zur Quantentheorie an. Es wird erklärt wie eine klassische Poisson*-Algebra als Grundlage eines zu quantisierenden Systems aufgebaut ist und warum die verschmierten Ashtekar-Variablen, die als Holonomien und Flüsse bezeichnet werden, die grundlegenden Variablen sind, aus denen alle weiteren Größen in der SQG gebildet werden können. Die Quantisierung der Holonomien und Flüsse führt auf den kinematischen SQG-Hilbertraum. Nach erfolgter Quantisierung der Holonomien und Flüsse werden die Zwangsbedingungen als Funktionen der Holonomien und Flüsse mittels Dirac-Quantisierung auf dem kinematischen Hilbertraum quantisiert. Als Zwischenschritt wird noch der Volumenoperator als Funktion der Holonomien und Flüsse, welcher eine eigenständige Bedeutung besitzt, aber auch in anderen zu quantisierenden Größen vorkommt, hergeleitet. Nacheinander werden die Zwangsbedingungsoperatoren auf die Zustände

des kinematischen Hilbertraums angewandt, um vom kinematischen zum physikalischen Hilbertraum zu gelangen.

Der folgende Teil III stellt ergänzend zur Dirac-Quantisierung aus Teil II die reduzierte Phasenraumquantisierung und deren Anwendung auf das Referenzmateriemodell mit vier Klein-Gordon-Skalarfeldern vor. Bei der Dirac-Quantisierung werden alle interessierenden Größen, insbesondere die Zwangsbedingungen aus der Hamiltonfunktion der ART, zunächst auf dem kinematischen Hilbertraum quantisiert, welcher bei vorkommenden Zwangsbedingungen nicht dem physikalischen Hilbertraum entspricht. Anschließend werden die Zwangsbedingungsoperatoren auf dem kinematischen Hilbertraum gelöst, um den physikalischen Hilbertraum zu erhalten, siehe das Vorgehen in Abschnitt 2. Hingegen wird bei der in Abschnitt 3 beschriebenen reduzierten Phasenraumquantisierung zu Beginn der Phasenraum der ART erweitert, in dem zur Einstein-Hilbert-Wirkung eine zusätzliche Materiewirkung addiert wird. Mit Hilfe der zusätzlichen Materie gelingt es die Zwangsbedingungen, wie in Abschnitt 3 und 4 erklärt, umzuschreiben [17, 18, 19] und auf dem klassischen Phasenraum ganz oder teilweise zu lösen. Durch die sogenannte Observablen-Abbildung [17, 18, 19, 20], beschrieben in Abschnitt 5, gewinnt man eichinvariante Größen, auch Dirac-Observablen genannt, welche eichinvariant unter einem Teil oder allen Eichtransformationen der ART, d.h. zeitlichen und räumlichen Diffeomorphismen, sind. Insbesondere erhält man eine Hamiltonfunktion, welche eine Entwicklung in Bezug auf eine Materievariable bzw. eines der Materiefelder beschreibt und für gewöhnlich als physikalische Hamiltonfunktion bezeichnet wird. Daher spricht man in diesem Zusammenhang auch von Referenzmaterie. Die Referenzmaterie nimmt die Rolle eines Beobachters ein, aus dessen Sicht das System beschrieben wird, siehe auch [21, 22]. Eine Klassifikation [23] bisher in der Literatur beschriebener Referenzmateriemodelle wird in Abschnitt 6 zusammengefasst. Im Anschluss an die Observablenabbildung wird versucht die klassischen Observablen, welche von den Referenzmaterie abhängen, zu quantisieren. Für den Fall, dass man die Wirkung von vier Klein-Gordon-Skalarfeldern zur Einstein-Hilbert Wirkung addiert, welches eine Verallgemeinerung der in [1, 24] beschriebenen Modelle darstellt, stellt sich dabei in Abschnitt 7 heraus, dass die sich ergebende physikalische Hamiltonfunktion nicht mit den Methoden der SQG quantisierbar ist. Dieses Ergebnis überrascht, da so ein Verhalten bisher nicht in der Literatur [1, 5, 23, 25, 26] erfasst ist und es sich um ein einfaches Referenzmateriemodell handelt. Dies zeigt zudem, dass es Modelle gibt welche Dirac quantisierbar sind, aber nicht mit der reduzierten Phasenraumquantisierung behandelt werden können und dient als Beispiel dafür, dass die beiden Quantisierungsmethoden zu sehr unterschiedlichen Resultaten führen können. Das Modell wird in den folgenden Abschnitten 8 und 9 durch die Einführung weiterer Freiheitsgrade verallgemeinert, mit dem Ergebnis, dass die mit Hilfe des verallgemeinerten Modells gewonnene Hamiltonfunktion mit Methoden der SQG quantisiert werden kann. Der so gewonnene physikalische Hamiltonoperator wird in Hinblick auf seine physikalischen Eigenschaften, insbesondere der Wirkung auf die als Spinnetzwerkfunktionen bekannten Basisfunktionen innerhalb der SQG und Algebraischen Quantengravitation, untersucht. Die Ergebnisse dieses Teils werden in Abschnitt 10 zusammengefasst.
Die mittels der vier verallgemeinerten Klein-Gordon-Skalarfeldern hergeleitete physikalische Hamiltonfunktion bzw. der zugehörige Operator aus Teil III teilt eine Eigenschaft mit vielen anderen in der Literatur befindlichen physikalischen Hamiltonfunktionen bzw. -operatoren: Er wird gebildet aus der Wurzel einer Hamiltondichte, welche wiederum „innere“ Wurzelfunktionen enthalten kann [1]. In diesem Zusammenhang wird auch von der „äußeren Wurzel“gesprochen. Die Wurzeln oder allgemeiner halbzahlige Potenzen innerhalb der Hamiltondichte finden sich für gewöhnlich in Polynomen von Holonomien und halbzahligen Potenzen von Flüssen und können mit den Methoden aus [4] behandelt werden, siehe dazu auch Abschnitt 11. Hingegen sind die Techniken aus [4] nicht direkt auf die äußeren Wurzeln

[1]Eine Ausnahme bildet der unter zur Hilfenahme von Gausschen Staubfelder [23] gewonnenen physikalischen Hamiltonoperator.

übertragbar.

In Teil IV wird die Fragestellung aufgegriffen, ob die semiklassische Störungstheorie beschrieben in [4] dahingehend erweitert werden kann, dass sie auch auf die äußeren Wurzeln anwendbar ist. Abschnitt 11 gibt eine kurze Einführung in die semiklassische Störungstheorie aus [4]. Zur Beantwortung der Frage der Erweiterbarkeit der semiklassischen Störungstheorie auf die äußeren Wurzeln wird in Abschnitt 12 das sogenannte Brown-Kuchař Staubmodell betrachtet, welches in einer Reihe von aufeinander folgenden Artikeln entwickelt wurde [25, 27, 28] und in [5] mittels reduzierter Phasenraumquantisierung quantisiert wurde. Der physikalische Hamiltonoperator im Brown-Kuchař-Staub-Modell ist von der Form her einfacher als der von uns bestimmte physikalische Hamiltonoperator für die verallgemeinerten Klein-Gordon-Felder und abgesehen von der äußeren Wurzel ähnlich zum Masterzwangsbedingungsoperator [29, 30], dessen semiklassischer Grenzwert in [3] in den Komplexifizierer-Kohärenten-Zuständen mit Hilfe der Methoden aus [4] berechnet wurde. Das Resultat des Versuchs die semiklassische Störungstheorie auf diesen physikalischen Hamiltonoperator zu erweitern ist, dass dies möglich ist, vorausgesetzt es lässt sich ein selbst-adjungierter Hamiltonoperator konstruieren und bestimmte Fluktuationen einer Näherung der Hamiltondichte unter der Wurzel klein genug sind. Es zeigt sich, dass in nullter Ordnung in $\hbar$ der Erwartungswert des Wurzel-Hamiltonoperators, oder bestimmter allgemeinerer halbzahliger Potenzen, in den Komplexifizierer-Kohärenten-Zuständen durch die Wurzel bzw. der halbzahligen Potenz aus dem Erwartungswert des physikalischen Hamiltondichteoperators in den Komplexifizierer-Kohärenten-Zuständen ersetzt werden kann. Jedoch führt das Vorgehen im Allgemeinen schnell auf technisch komplizierte und aufwendige Ausdrücke, so dass ein anderer Ansatzpunkt darin liegt die funktionale Form der Hamiltonoperatoren mehr in die Konstruktion der semiklassischen Zustände einzubeziehen, als dass für die Komplexifizierer-Kohärenten-Zustände der Fall ist. Die Ergebnisse aus Teil IV sind unter den oben genannten Voraussetzungen auch auf andere physikalische Hamiltonoperatoren übertragbar. Die Resultate werden in Abschnitt 13 diskutiert.

Um diesen Ansatz zu verfolgen, werden in Teil V Methoden untersucht die Wurzel- oder allgemeiner fraktionale Hamiltonoperatoren zu handhaben, insbesondere werden Konstruktionsverfahren für Zustände, die diese funktionale Form besser berücksichtigen, gesucht. Zu diesem Zweck wird ein quantenmechanisches Spielzeugmodell betrachtet, welches aus der Wurzel des Hamiltonoperators für den zeitunabhängigen harmonischen Oszillator besteht. In diesem Teil bezieht sich der Ausdruck Wurzelhamiltonfunktion bzw. -operator stets auf dieses Spielzeugmodell. Da die gesuchten Zustände auf Operatoren angewendet werden sollen mit dem Ziel im Erwartungswert den klassischen Wert, wenigstens näherungsweise im Limes kleiner Quantenfluktuationen, zu reproduzieren, handelt es sich dabei um semiklassische Zustände. Nach einer kurzen Motivation und Übersicht über die in Teil V behandelten Methoden in Abschnitt 14, wird in Unterabschnitt 14.1 detailliert erklärt welche definierenden Eigenschaften semiklassische und kohärente Zustände aufweisen [9, 31, 32, 33, 34]. Anschließend werden in Unterabschnitt 14.2 die Eigenschaften des harmonischen Oszillators zusammengefasst [35, 36, 37, 38] und die verschiedenen Konstruktionsverfahren für die kohärenten Zustände des harmonischen Oszillators erörtert, welche als Inspirationsquelle für viele Konstruktionsverfahren allgemeinerer Systeme dienen. Die drei Konstruktionsverfahren für kohärente Zustände im Falle des harmonischen Oszillators lassen sich beschreiben als: 1.) Ein kohärenter Zustand ist ein Eigenzustand des Vernichtungsoperators, 2.) Ein kohärenter Zustand ist das Resultat der Anwendung des Verschiebungsoperators auf den Grundzustand und 3.) Ein kohärenter Zustand ist ein Zustand minimaler Unschärfe. Im Falle des harmonischen Oszillators führen alle drei Konstruktionsverfahren zu äquivalenten Zuständen. Dies trifft im Allgemeinen nicht mehr zu [39].
Zunächst werden zwei Verfahren vorgestellt, mit denen es nicht gelungen ist geeigneten neue semiklassischen Zustände für die Wurzeloperatoren zu konstruieren, die allerdings hilfreich

waren um herauszufinden worauf bei einem Konstruktionsverfahren für die neuen semiklassischen Zustände zu achten ist. Die inverse Thiemannidentität in Abschnitt 15, bei der es darum geht die Wurzelfunktion bei der Herleitung der Bewegungsgleichungen in der klassischen Beschreibung umzuschreiben ist motiviert durch die sogenannte Thiemannidentität, welche bei der Quantisierung der Dynamik der SQG angewandt wird. Dabei erlaubt die Thiemannidentität eine inverse Wurzelpotenz einer Phasenraumfunktion durch entsprechende Poissonklammern zu ersetzen. Hier führt die inverse Thiemannidentität auf einen harmonischen Oszillator mit einer modifizierten Frequenz. Das gewonnene Modell wird quantisiert, aber dabei wird die modifizierte Frequenz als Funktion der klassischen Energie für die Wurzel aus der Hamiltonfunktion des harmonischen Oszillators betrachtet. Für das so gewonnene Modell können neue Erzeugungs- und Vernichtungsoperatoren angegeben werden, die als Resultat einer Bogoliubov-Transformation aufgefasst werden können. Als Eigenzustände des neuen Vernichtungsoperators dienen sogenannten komprimierte (squeezed) Zustände. Allerdings zeigt sich bei der Berechnung des Erwartungswertes des mit Hilfe der inversen Thiemannidentität gewonnenen Operators in diesen Zuständen, dass der Erwartungswert nicht den zugehörigen klassischen Wert für den Operator approximiert. Daher sind diese Zustände und die inverse Thiemannidentität für unsere Zwecke ungeeignet.

Eine Verallgemeinerung der Erzeugungs- und Vernichtungsoperatoren findet sich auch in Abschnitt 16, wo das Verfahren aus [40, 41] zur Konstruktion von sogenannte Phasenoperatoren und Phasenzuständen erläutert und modifiziert wird mit dem Ziel es auf den Wurzelhamiltonoperator anzuwenden. Das Verfahren diente ursprünglich dazu Zustände für bestimmte Erweiterungen der Weyl-Heisenberg-Algebra zu konstruieren. Die konstruierten sogenannten Phasenzustände sind Eigenzustände des nicht unitären Phasenraumoperators. Allerdings sind sie keine Eigenzustände zu dem dort definierten Vernichtungsoperator. Das Verfahren wird modifiziert, um Zustände für unseren Wurzelhamiltonoperator zu erhalten. Allerdings erfüllen diese Zustände nicht die Erwartungswertreproduktion des klassischen Werts für den Wurzelhamiltonoperator und sind somit keine semiklassischen Zustände für diesen Operator. Eine eventuell nützliche Eigenschaft ist jedoch, dass sie zeitlich stabil unter dem Wurzelhamiltonoperator als Entwicklungsoperator sind.

Dieses zeitliche Entwicklungsverhalten zeigt sich auch bei den im nachfolgenden Abschnitt 17 nach einem Verfahren von Klauder et al., siehe z.B. [33, 42], konstruierten Zuständen. Deren Konstruktion fußt auf den Wirkungs-Winkel-Variablen (action angle variables) und nicht auf den Orts- und Impulsvariablen. Klassisch wird ein Übergang von den Orts- und Impulsvariablen in die Wirkungs-Winkel-Variablen durch eine kanonische Transformation erreicht. Für den Fall der Wurzel des harmonischen Oszillators kann man auch dieses System in die Wirkungs-Winkel-Variablen umschreiben. Dies ist im Allgemeinen jedoch nicht ohne Weiteres möglich. Unter einigen Annahmen lassen sich kohärente Zustände nach Klauder für den Wurzelhamiltonoperator konstruieren. Diese erfüllen per Konstruktionsverfahren die Eigenschaft, dass sie den klassischen Ausdruck für die betrachtete Hamiltonfunktion, wenn man den Erwartungswert des Operators berechnet, reproduzieren und sind gemäß Klauders Definition zeitlich stabil.

Ein allgemeineres auf Lie-Gruppeneigenschaften beruhendes Konstruktionsverfahren ist die in Abschnitt 18 beschriebene und in [31, 43, 44, 45, 46] entwickelte Komplexifizierermethode. Allerdings ist diese nicht für unsere Wurzelhamiltonfunktion geeignet, da in der Konstruktion als Ausgangslage nur ganzzahlige Potenzen von Orts- und Impulsoperatoren, sowie Polynome aus diesen berücksichtigt werden. Die Methode wird dennoch vorgestellt, da für die semiklassische Störungstheorie in Teil IV Komplexifizierer-Kohärente-Zustände verwendet wurden. Durch die Rechnungen in Teil IV hat sich wie oben erläutert auch noch einmal gezeigt, dass diese Zustände nicht an die fraktionalen Hamiltonoperatoren angepasst sind. Eine neuere Alternative zu den Komplexifizierer-Kohärenten-Zuständen sind die in [47] beschriebenen Zustände, deren Konstruktion jedoch ebenfalls nicht auf Wurzeloperatoren ausgelegt wurde.

Im folgenden Abschnitt 19 wird die algebraische Konstruktion [32, 48, 49, 50, 51, 52]

kohärenter Zustände eingeführt und es werden die benötigte Definitionen zu Algebren und deren Eigenschaften zusammengetragen. Dieses Verfahren ist für alle Systeme anwendbar für die eine sogenannte spektrumerzeugende Algebra bekannt ist.
Um eine spektrumerzeugende Algebra zu erhalten werden in Abschnitt 20 Definitionen aus verschiedenen Quellen [53, 54, 55] für die spektrumerzeugende Algebra, Implikationen in Bezug auf Lie Algebren und Verfahren wie eine spektrumerzeugende Algebra bestimmt werden kann zusammengetragen.
Im Folgenden werden in Abschnitt 21 die verschiedenen Begriffe von Stabilität [31, 37, 40, 42], welche uns bisher im Teil V begegnet sind, rekapituliert und der für die hier betrachteten Verfahren allgemeinste Stabilitätsbegriff daraus extrahiert. Dann wird dieser Stabilitätsbegriff mit der algebraischen Konstruktion kombiniert, um zu sehen welche Bedingungen und Zusammenhänge für die Stabilität der Zustände eines Systems, welche mit Hilfe der algebraischen Konstruktion konstruiert werden, sich bereits aus den algebraischen Eigenschaften des Systems ergeben. Neben Resultaten aus dieser Arbeit werden ebenfalls bekannte Resultate zum Thema der Stabilität semiklassischer Zustände [31, 56, 57, 58, 59, 60, 61] betrachtet, um zu sehen unter welchen Bedingungen ein Zustand stabil bleibt und was passiert, wenn kleine zu Instabilitäten führende Terme zur Hamiltonfunktion hinzugefügt werden. Die Überlegungen zur Stabilität und die Definitionen der spektrumerzeugenden Algebra führen zu dem Resultat, dass im Falle der Wurzelhamiltonfunktion entweder nach einer Algebra gesucht werden sollte welche isomorph zur Weyl-Heisenberg-Algebra ist oder die Weyl-Heisenberg-Algebra selbst als spektrumerzeugende Algebra verwendet werden kann.
In Abschnitt 22 wird die Idee einer effektiven Hamiltonfunktion aus Abschnitt 15 als Ersatz für die Wurzelhamiltonfunktion wieder aufgegriffen. Dazu wird ein erweiterter Phasenraum mit einer Zeitvariablen t und dem zugehörigen kanonisch konjugiertem Impuls p_t betrachtet, indem die Wurzelhamiltonfunktion oder eine allgemeinere fraktionale Hamiltonfunktion als Teil einer Zwangsbedingung formuliert werden kann. Mit Hilfe der sogenannten dualen Euler-Reskalierung, welche in diesem Zusammenhang eingeführt wird, ist es möglich t und p_t zu transformieren und die Zwangsbedingung dann nochmals so umzuschreiben, dass sie wieder die Hamiltonfunktion des harmonischen Oszillators ohne halbzahlige Potenzen enthält. Die Idee nach einer Transformation für den Zeitparameter zu suchen geht zurück auf unsere Versuche die Kumei Methode [62] in Abschnitt 20.2.2 anzuwenden. Die so gewonnene Hamiltonfunktion kann als effektive Hamiltonfunktion für das Problem der fraktionalen Hamiltonfunktionen aufgefasst werden. Statt der halbzahligen Potenz der Hamiltonfunktion, haben wir jetzt eine halbzahlige Potenz des Impulsoperators p_t. Halbzahlige Potenzen des Impulsoperators können, wie in [63] gezeigt wurde, unter Verwendung von Kummerfunktionen gut durch die Standardzustände des harmonischen Oszillators approximiert werden. Damit und gemäß der Methode in [64] werden physikalische kohärente Zustände für Systeme mit Zwangsbedingungen konstruiert und ihre Eigenschaften analysiert. Man beachte, dass in [64] nur Zwangsbedingungen betrachtet werden die entweder linear oder quadratisch von den Phasenraumvariablen abhängen. In dieser Arbeit jedoch wurde die Prozedur erweitert und es wurde gezeigt, dass die Methode auch auf Zwangsbedingungen angewendet werden kann die halbzahlige Potenzen der Phasenraumvariablen enthalten. Die physikalischen kohärenten Zustände unterscheiden sich von den kinematischen kohärenten Zuständen durch eine Einschränkung ihrer Phasenraumlabel, welche sich aus der betrachteten Zwangsbedingung ergibt. Daher wird die Einschränkung des Phasenraumlabels bereits bei der Konstruktion der kohärenten Zustände in Abschnitt 23 berücksichtigt, wodurch die Anpassung der Zustände an die fraktionalen Hamiltonfunktionen bzw. -operatoren erfolgt.
In Abschnitt 23 werden verallgemeinerte kohärente Zustände konstruiert, welche auf fraktionalen Poisson-Verteilungen aufbauen. Zunächst wird die in [65, 66] eingeführte Konstruktion von kohärenten Zuständen für fraktionale Poisson-Verteilungen vorgestellt. In [66] wurde gezeigt, dass die kohärenten Zuständen für fraktionale Poisson-Verteilungen normierbar sind und eine Zerlegung des Einheitsoperators besitzen. Allerdings ist im dortigen Beweis ein Fehler unterlaufen, der in einer ähnlichen Rechnung in diesem Abschnitt korrigiert werden

konnte. Da diese Zustände jedoch noch nicht die gewünschte Eigenschaft erfüllen, Eigenzustände des Vernichtungsoperators zu sein, wird die Konstruktion modifiziert. Eine leichte Modifikation führt dazu, dass sie Eigenzustände des Vernichtungsoperator werden und die zugrundeliegenden Operatoren damit auch die Weyl-Heisenberg-Algebra erfüllen. Zusätzlich wird gezeigt, dass diese Zustände normierbar sind und eine Zerlegung des Einheitsoperators besitzen, d.h. übervollständig sind. Die verallgemeinerten Zustände können als die Standardzustände des harmonischen Oszillators mit modifizierten Labeln aufgefasst werden, welche an den betrachteten fraktionalen Hamiltonoperator angepasst sind. Mit Hilfe dieser Zustände kann der Operator des harmonischen Oszillators als ein effektiver Hamiltonoperator für die Berechnung von semiklassischen Erwartungswerten aufgefasst werden. Um die Zerlegung des Einheitsoperators zu zeigen, muss der Maßraum erweitert werden, was das Problem mit dem Beweis von Laskin in [66] löst, aber neue Fragen bzgl. der Verbindung zu den klassischen Phasenraumlabeln aufwirft. Zunächst beeinflusst die Erweiterung des Maßraums nur die klassischen Phasenraumlabel, jedoch sind diese Label mit Observablen verknüpft, welche in der Quantentheorie zu Operatoren werden. Diese Fragen können dadurch umgangen werden, dass das Problem nicht weiterhin in der üblichen Schrödinger Darstellung, sondern im Hilbertraum der quasi-periodischen Funktionen betrachtet wird. Eine Folge davon ist allerdings, dass der harmonische Oszillator ausgedrückt durch den Anzahloperator nicht als Operator auf diesem Hilbertraum existiert. Um Fortzufahren bedarf es daher bei diesem Vorgehen mehr Aufwand um die Zerlegung des Einheitsoperators zu zeigen. Glücklicherweise gibt es jedoch in der Literatur bereits eine Vielzahl von Resultaten bezüglich des polymer harmonischen Oszillators [67, 68, 69, 70] auf die hier zurückgegriffen werden kann. Die Resultate hieraus werden in [71] veröffentlicht werden. Schließlich werden die Ergebnisse aus Teil V in Abschnitt 24 zusammengefasst und diskutiert.

Teil VI fasst wichtige Folgerungen aus allen Teilen grob zusammen und bietet einen Ausblick auf zukünftige Forschungsthemen. Für detaillierte Diskussionen der Ergebnisse der einzelnen Teile sei auch noch einmal auf die Abschnitte 10, 13 und 24 verwiesen.

Executive Summary

Semiclassical Dynamics of Loop Quantum Gravity

The subject of this work is the analysis and improvement of semiclassical techniques within Loop Quantum Gravity (LQG) with the intention to check whether the operators of interest reassemble their classical counterparts in the semiclassical limit or not. Prior work concerning these issues in the context of semiclassical perturbation theory making use of so-called complexifier coherent states can be found in [2, 3, 4, 5]. What is new in this work is on the one hand the class of considered operators under semiclassical aspects, which are denoted as physical Hamiltonian operators, and on the other hand that a variety of techniques beyond semiclassical perturbation theory is examined. Physical Hamiltonians in the context of General Relativity (GR) can result from the addition of matter actions to the gravitational action, the Einstein-Hilbert action. Then a physical Hamiltonian is usually, at least partly, quantized by performing a so-called reduced phase space quantization that leads to the physical Hamiltonian operator. During the cause of this work it was discovered that there exist models which according to the kind of added matter actions are Dirac quantizable, see part II, but not necessarily quantizable via reduced phase space quantization, see part III. Subject to the functional form of the physical Hamiltonian operator it can technically become arbitrary complex to transfer the semiclassical techniques developed in [4] to the physical Hamiltonian operators and requires a more precise analysis of the problem as can be found in the literature so far. Therefore, within the scope of this thesis it is tried to find or develop new semiclassical and alternative techniques, especially new semiclassical states, which incorporate the functional form of the physical Hamiltonian operators.

Part I explains the motivation for and structure of the following work.

Part II describes the development from GR to the formulation of LQG [6, 7, 8, 9, 10, 11, 12, 13]. Starting from Einstein's equations in section 1 it is first shown how they can be obtained from the variation of the Einstein-Hilbert action. The Einstein-Hilbert action includes by definition the Lagrange function of GR which is used in the upcoming. After an introduction to the ADM decomposition [14], which is visualized by a split into temporal and spatial components, a Lengendre transformation from the Lagrangian to the Hamiltonian formulation of GR is performed. As a result it turns out that the Hamiltonian of GR consists of constraints only, which are generators for temporal and spatial diffeomorphisms; these are the gauge transformations of GR. It is continued with the derivation and discussion of the constraint algebra that is usually referred to as hypersurface deformation algebra [15] or Dirac algebra [16]. At the end of section 1 the transformation from the position and momentum phase space variables to the new Ashtekar variables, which are fundamental for the following quantization procedure, is described. Section 2 then continues with the quantization of GR formulated in Ashtekar variables. It is explained how the classical Poisson* algebra of a physical system can be used as a starting point for a quantization of this system. Furthermore it is explained why the smeared Ashtekar variables, which are denoted as holonomies and fluxes, are the fundamental variables from which all further quantities in LQG can be composed. After the quantization of the holonomies and the fluxes, the constraints on the kinematical Hilbert space are quantized via Dirac quantization. In an intermediate step it is also shown how the quantization of the volume operator, which has a meaning on its own, but is also used in the quantization of other quantities, can be performed. Step by step the different constraints on the kinematical Hilbert space are solved to finally arrive at the physical Hilbert space of LQG.

In the following part III supplementary to the Dirac quantization of part II the reduced phase space quantization is discussed and especially its application to a model with four Klein-Gordon scalar fields as reference matter. In the case of Dirac quantization all quan-

tities of interest, especially the constraints in the Hamiltonian of GR, are quantized on the kinematical Hilbert space which will be different from the physical Hilbert space if constraints occur. Afterwards the constraint operators have to be solved on the kinematical Hilbert space to obtain the physical Hilbert space, for an example see the procedure in section 2. On the contrary in case of reduced phase space quantization as described in section 3, one starts with enlarging the phase space of GR by adding an additional matter action to the Einstein-Hilbert action. With the help of the additional reference matter it is possible to rewrite the constraints [17, 18, 19], as explained in section 3 and 4, and to solve them completely or partially on the classical phase space. By application of the so-called observable map [17, 18, 19, 20], as described in section 5, gauge invariant quantities denoted as Dirac observables are obtained, which are gauge invariant under some or all gauge transformations of GR, i.e. temporal and spatial diffeomorphisms. In particular a Hamiltonian whose evolution can be described with respect to a chosen matter variable or field, which is usually denoted as physical Hamiltonian, can be constructed. Therefore, one usually denotes this matter as reference matter. The reference matter plays the role of an observer from whose perspective the physical system in consideration is described, see also [21, 22]. A classification of the reference matter models [23] considered in the literature so far is summarized in section 6. After the application of the observable map, it is tried to quantize the classical reference matter dependent observables. For the case of adding the action of four Klein-Gordon scalar fields to the Einstein-Hilbert action in section 7, which is a generalization of the models in [1, 24], it turns out that the resulting physical Hamiltonian cannot be quantized by the methods of LQG. This result is surprising, since such an behaviour has not been observed by other models considered in the literature [1, 5, 23, 25, 26] so far and the reference matter model in consideration is quite simple. Additionally, this shows that there exist models which can be quantized by Dirac quantization but not by reduced phase space quantization and serves as an example for the case that both quantization methods can lead to differing results. This model is generalized in sections 8 and 9 by introducing additional degrees of freedoms which results in a generalized model that can be quantized by the methods of LQG. The physical properties of the resulting physical Hamiltonian operator are analyzed, especially the action on the spin network functions that are basis states in the context of Loop or Algebraic Quantum Gravity. Our conclusions for this part can be found in section 10.
The physical Hamiltonian or the related operator which was derived with the help of the four generalized Klein-Gordon scalar fields in part III has something in common with most of the physical Hamiltonians appearing in the literature. It can be expressed by a square root of a Hamiltonian density, which itself can include "inner" square root functions. In this context the term "outer square root" is introduced [2]. Square roots or more general fractional powers that occur inside of the Hamiltonian density are usually contained in polynomials of holonomies and fractional powers of fluxes and can be treated by the methods of [4], compare also section 11. However, one can not apply the methods of [4] to the outer square roots directly.

In part IV as a starting point the question whether it is possible to generalize the semiclassical perturbation theory described in [4] to handle outer square roots is considered. Section 11 gives a short review on semiclassical perturbation theory developed in [4]. To answer the question whether semiclassical perturbation theory can be extended to the outer square roots, in section 12 the so-called Brown-Kuchař dust model which was derived in a series of articles [25, 27, 28] and quantized in [5] via reduced phase space quantization is examined. The form of the physical Brown-Kuchař dust Hamiltonian operator is simpler than the form of the physical Hamiltonian operator derived from the generalized four Klein-Gordon scalar field model and except from the outer square root similar to the Master constraint operator derived in [29, 30] whose semiclassical limit in complexifier coherent states was calculated in

[2] An exception is the physical Hamiltonian operator obtained with the help of Gaussian dust in [23].

[3] by the methods of [4]. The approach to extend semiclassical perturbation theory to this physical Hamiltonian operator led to the insight that this is possible under the conditions that one can construct a self-adjoint operator and certain fluctuations of an approximation of the Hamiltonian density under the square root are small. It is found that to lowest order in $\hbar$ the expectation value of the square root or more general certain fractional power Hamiltonian operators in complexifier coherent states can be replaced by the square root or fractional power respectively of the expectation value of the Hamiltonian density operator in complexifier coherent states. However, in general our generalization of semiclassical perturbation theory ends in technically complex and elaborate expressions. Therefore, the idea to incorporate the functional form of the Hamiltonian operator more in the construction of semiclassical states than it is done in the construction of the complexifier coherent states is taken as a different starting point. The methods in part IV can also be applied to a wider class of physical Hamiltonian operators assuming that the conditions mentioned above still hold. The results are discussed in section 13.

To resolve this issue, in part V methods to handle square root or more general fractional Hamiltonian operators are analyzed, in particular different construction methods for states which are better adapted to the functional form of these Hamiltonian operators are considered. For this purpose the square root of the Hamiltonian operator for the time-independent harmonic oscillator is used as a quantum mechanical toy model. In the following when the term square root Hamiltonian is used it refers to this toy model. Since one wants to calculate the expectation values of operators in these states with the aim to reproduce their classical values, at least approximately in the limit of small quantum fluctuations, those states are denoted as semiclassical states. After a short motivation and overview over the methods used in part V in section 14, the defining properties of semiclassical and coherent states are described in section 14.1 in detail [9, 31, 32, 33, 34]. This is followed by a summary of the properties of the harmonic oscillator coherent states [35, 36, 37, 38] and the different construction methods for them in section 14.2. These construction methods serve as an inspiration for many other more general construction methods for coherent states. They can roughly be characterized into three different types: 1.) a coherent state is an eigenstate of the annihilation operator, 2.) a coherent state is the result of the application of the displacement operator to a ground state, 3.) a coherent state is a state of minimal uncertainty. In case of the harmonic oscillator all three construction methods lead to equivalent states. This does not apply to the general case [39].
First two methods which turned out to be unsuitable for the construction of new semiclassical states for the square root Hamiltonian operator are presented, nevertheless they proved to be helpful in pointing out what should be paid attention for in the construction of new semiclassical states. The inverse Thiemann identity in section 15, which is introduced to rewrite the square root on the classical level in the derivation of the equations of motion, is motivated by the so-called Thiemann identity, which is applied in the quantization of the dynamics of LQG. There with the help of the Thiemann identity it is possible to substitute an inverse fractional power of a phase space function by Poisson brackets. Here the inverse Thiemann identity leads to a harmonic oscillator with a modified frequency. This model is quantized, however the modified frequency is considered as a function of the classical energy for the square root of the harmonic oscillator Hamiltonian. It is possible to define new annihilation and creation operators for the resulting model which can be seen as the result of a Bogoliubov transformation. Eigenstates of the new annihilation operator are given in form of so-called squeezed states. However, the expectation value of the so-gained operator in squeezed states does not approximate the classical value corresponding to the operator. Consequently, these states and the inverse Thiemann identity are not appropriate for our purpose.
Another generalization for annihilation and creation operators can be found in section 16, where a procedure from [40, 41] to construct so-called phase operators and phase states

with the aim to apply the procedure to the square root Hamiltonian operator is considered and modified. Originally, the procedure was introduced to construct states for a certain generalization of the Weyl-Heisenberg algebra. The obtained, so-called phase states are eigenstates of the non-unitary phase operator. Unfortunately, they are no eigenstates of the generalized annihilation operator. The procedure is modified to obtain states that are adapted to the square root Hamiltonian operator. However, the expectation value of the square root Hamiltonian in these states does not reproduce the expected classical value, so these states are no semiclassical states for the square root Hamiltonian operator. Despite that they might be useful, if one considers the time-evolution with respect to the square root Hamiltonian operator, since they are stable under this evolution.

In section 17 a similar time-evolution behaviour with respect to the square root Hamiltonian operator can be observed when states following a method introduced by Klauder et al., see for example [33, 42], are constructed. This construction is based on the so-called action angle variables instead of position and momentum variables. On the classical level one can perform a canonical transformation to come from the position and momentum variables to the action angle variables. For the case of the square root of the harmonic oscillator this system can be formulated in terms of action angle variables and coherent states in the sense of Klauder et al. are constructed. This might not be possible in the general case. To be able to construct Klauder coherent states for the square root Hamiltonian, some assumptions have to be made. The expectation value of the square root Hamiltonian operator in these Klauder coherent states reproduces the classical value by construction and the states are temporally stable in the sense of Klauder.

A more general construction principle based on the properties of Lie groups is the complexifier method described in section 18 and developed in [31, 43, 44, 45, 46]. However, this method cannot be applied to our square root Hamiltonian due to the point that the construction of the complexifier coherent states is adapted to integer powers of position and momentum operators and polynomials of them. Nevertheless, this method is discussed, since the complexifier coherent states were used explicitly in semiclassical perturbation theory in part IV. That the complexifier coherent states are by construction not adapted to the fractional Hamiltonians is reflected by our calculations in part IV as discussed above. A recent alternative to the complexifier coherent states are the states constructed in [47], however their construction is also not designed to handle square root Hamiltonian operators.

In the following section 19 the algebraic construction [32, 48, 49, 50, 51, 52] for coherent states is introduced and required definitions about algebras and their properties are collected. This method can be applied to all systems whose so-called spectrum generating algebra is known. To obtain the spectrum generating algebra in section 20 several definitions concerning the spectrum generating algebra from different sources [53, 54, 55], implications related to Lie algebras as well as possibilities to find spectrum generating algebras are reviewed.

Subsequently, in section 21 the various notions of stability [31, 37, 40, 42] which occured in part V are collected and from this the most common notion of stability for the procedures in this work is extracted. Then this notion of stability is combined with the algebraic construction to find out which conditions and correlations concerning the stability of states of a physical system can already be derived from its algebraic properties. In addition to our results from this work also known results concerning the stability of semiclassical states [31, 56, 57, 58, 59, 60, 61] are taken into account to find out under which circumstances a state is stable and what will happen, if small perturbations are added to the Hamiltonian.

Finally, our considerations regarding stability combined with the definitions of spectrum generating algebras lead us to the conclusion that in case of the square root Hamiltonian one should either search for an algebra which is isomorphic to the Weyl-Heisenberg algebra or take the Weyl-Heisenberg algebra itself as a spectrum generating algebra.

In section 22 the idea from section 15 of finding an effective Hamiltonian equivalent for our square root Hamiltonian is picked up. For this purpose an enlarged phase space containing an additional time variable t and its canonically conjugated momentum p_t, in which the

square root Hamiltonian or a more general fractional Hamiltonian can be understood as part of a constraint, is constructed. By application of the so-called dual Euler rescaling, which will be explained in this context, it is further possible to transform t and p_t and to rewrite this constraint to include a harmonic oscillator Hamiltonian without fractional powers. The idea to search for a transformation of the time parameter was inspired by the Kumei method [62] in section 20.2.2. The so gained Hamiltonian can be seen as an effective Hamiltonian for fractional Hamiltonians. Instead of having a fractional Hamiltonian the fractional power is moved to the momentum operator p_t. Fractional powers of the momentum operator can be well approximated by the standard harmonic oscillator coherent states using Kummer functions as shown in [63]. With this and following the method given in [64] physical coherent states for systems with constraints are constructed and their properties are investigated. Notice that the work in [64] considers only constraints with an either linear or quadratic dependence on the elementary phase space variables. However, in this work the framework is enlarged and it is shown that it can also be applied to constraints that involve fractional powers of the elementary phase space variables. The physical coherent states differ from the kinematical ones by a restriction on their label set that is determined by the form of the constraint under consideration. Consequently, in section 23 this restriction on the labels is already incorporated into the construction of the coherent states which makes them well suited for fractional powers of the Hamiltonian.
In section 23 generalized coherent states based on fractional Poisson distributions are constructed. First a construction for coherent states for fractional Poisson distributions introduced in [65, 66] is recalled. In [66] it was shown that the coherent states for fractional Poisson distributions are normalized and satisfy a resolution of identity, however there was a mistake in the proof in [66] which is fixed in the similar calculations which are performed in this section. The construction in [66] is modified, since these states should be eigenstates of the annihilation operator. A slight modification makes them eigenstates of the annihilation operator and therefore the algebra of the underlying operators is simply the Weyl-Heisenberg algebra. Additionally, it was shown that these states are normalized and satisfy a resolution of identity.

The generalized states can be understood as standard coherent states of the harmonic oscillator but with labels that have been adopted to the fractional Hamiltonian under consideration. Given these states the standard harmonic oscillator Hamiltonian operator can be considered as a kind of effective Hamiltonian operator for the computation of the semiclassical expectation values. To show the resolution of identity for these generalized coherent states the measure space has to be enlarged which solves the issue in the proof by Laskin in [66] but brings up new questions concerning the relation to the classical labels. First this affects only the range for the classical labels, however these labels are associated with observables that become operators in the corresponding quantum theory. These questions can be circumvented if one no longer work with the usual Schrödinger representation but consider the Hilbert space of quasi-periodic functions. However, a consequence of this step is that the harmonic oscillator Hamiltonian written in terms of the number operator cannot be implemented as an operator on that Hilbert space. This requires more work before a proof of the resolution of identity can be performed in this framework but fortunately there exits already various results in the literature on the polymerized harmonic oscillator [67, 68, 69, 70] that can be applied here. The results out of these considerations will be published in [71]. Finally, the conclusions for part V are summarized in section 24.

Part VI roughly summarizes the main results from all parts and gives an outlook for future research. For a detailed discussion of the results of each part the reader is referred to sections 10, 13 and 24.

Part I
Motivation

In this work we consider semiclassical techniques in the context of Loop Quantum Gravity (LQG) and quantum mechanical toy models with the aim to understand whether the operators resulting from quantization procedures reassemble their classical counterparts as functions on a phase space in General Relativity (GR) or classical mechanics in the semiclassical limit.

In part II we display the standard techniques of Loop Quantum Gravity to get familiar with the classical formulation of General Relativity and its Dirac quantization in the context of Loop Quantum Gravity in section 1 and section 2. We begin with the Einstein field equations and explain the meaning of their components to capture the meaning of GR. Next we show that they can be obtained from the variation of the Einstein-Hilbert action which also gives us the Lagrangian formulation of GR. For the reason that we completely want to understand the LQG foundations and since in the literature this is often held shortly, we display the Legendre transformation to get from the Lagrangian formulation to the Hamiltonian formulation which leads to a Hamiltonian consisting only of constraints, as well as the calculation of the constraint algebra in detail. With the purpose to gain a deep understanding of how LQG developed to its current state, we also rigorously explain the introduction of the so-called Ashtekar variables and their quantization, respectively the quantization of their smeared analogues, leading to the kinematical LQG Hilbert space. To make things complete, we formulate the constraints in terms of the quantized smeared Ashtekar variables and review their solution one after another to transition from the kinematical to the physical LQG Hilbert space.

The next part III deals with the reduced phase space quantization of four Klein-Gordon scalar fields. Reduced phase space quantization brings a physical meaning to the constraints which make up the GR Hamiltonian by the introduction of an observer represented by additional matter actions added to the Einstein-Hilbert action. It is explained in section 3 what reduced phase space quantization in contrast to Dirac quantization is and what advantages and disadvantages both techniques have. As a preparation for the upcoming calculations in the part III some mathematical and physical definitions concerning constraints and observables are introduced in sections 4 and 5. Section 6 provides an overview and a classification of existing matter reference models. The interest in the reduced phase space quantization with four Klein-Gordon scalar fields as reference matter, discussed in section 7, arose due to two points: First it is a generalization of the model in [1], where one scalar field is introduced to reduce the phase space with respect to the Hamiltonian constraint. Second four Klein-Gordon scalar fields are simple compared to other matter reference fields used for reduced phase space quantization [23, 25, 28]. However, the outcome of the calculations is quite a surprise because in the first obvious ansatz the result was that the model after performing the phase space reduction is not quantizable using standard LQG techniques. By performing two generalization steps in sections 8 and 9, we arrived at a model in section 9 which includes four Klein-Gordon scalar fields plus three additional degrees of freedom and can be quantized. A detailed summary of the results is given in section 10.

Many physical Hamiltonian operators obtained from reduced phase space quantization contain square roots out of a Hamiltonian density. To approximate expectation values of fractional powers of the LQG volume operator and to justify the calculation of the semiclassical limit of the master constraint operator in [3] semiclassical perturbation theory was introduced in [4] which main techniques and results are summarized in section 11. We follow up the ideas from [4] in section 12 with the aim to approximately calculate the expectation values of physical Hamiltonian operators containing outer square roots in complexifier coherent states. From the results of section 12 we conclude in section 13 that the standard complexifier coherent states are not well-

adapted to the functional form of the physical Hamiltonian operators containing outer square roots.
This gives rise to the question whether there exists possibilities to construct semiclassical states which are better adapted to the functional form of the physical Hamiltonian operators. For the reason that the physical Hamiltonian operators are rather complex and we want to find out how to adapt the semiclassical states to the functional form of an operator, we consider quantum mechanical toy models instead. As a toy model we choose the square root or more general fractional powers of the standard harmonic oscillator operator, shortly denoted as square root or fractional Hamiltonian operators.
Part V exactly picks up the challenge to construct new semiclassical states for the square root or more general fractional powers of the harmonic oscillator as well as in some cases for polynomials which is due to the fact that we first thought about expanding the square root on the classical level. Additionally, we are interested in the time-evolution and stability of semiclassical states, since in this work we also want to consider semiclassical dynamics. For clarification we first explain in section 14.1 what we mean by a semiclassical state and what additional properties make a semiclassical state also a coherent state and how we define the semiclassical limit. Since the harmonic oscillator and its three possible construction principles for coherent states still are the source and inspiration for the construction of semiclassical or coherent states for all other kinds of physical systems, we shortly summarize the form, properties and construction of coherent states for the harmonic oscillator in section 14.2. When we follow the path of constructing new semiclassical states we come to methods which are concerned with finding new generalized annihilation and creation operators as in sections 15, 16, section 18 and appendix H.1 in which the Hamiltonian operator can be factorized. The generalized annihilation operators might be used to construct coherent states via the annihilation operator eigenstate approach.

As a first idea we want to construct a kind of effective Hamiltonian. Therefore, in section 15 we introduce a technique we denote as the inverse Thiemann identity to eliminate the square root on the classical level which leads to a harmonic oscillator with a modified frequency depending on the square root Hamiltonian. We perform a "semiclassical" quantization, where we consider the square root Hamiltonian occurring in the modified frequency as classical energy of the system and see that its semiclassical states are squeezed states, but no appropriate semiclassical states for the square root Hamiltonian. The states considered in section 16 are no semiclassical states for the square root Hamilton operator in the sense explained at the beginning of part V, however they are stable under time-evolution with respect to the square root Hamiltonian. Interestingly, some ideas of section 16 concerning the evolution properties of the states go over into the construction of Klauder coherent states in section 17. Though, there one uses instead of the position and momentum variables, respectively operators, a formulation in terms of action-angle-variables and the resulting states are coherent states in the sense of section 14.1. The methods introduced to construct coherent states so far, critically depend on the system in consideration. We want more general, mathematical construction principles. One such principle is the method to generate so-called complexifier coherent states explained in section 18 based on properties of the underlying physical group and the annihilation operator construction principle. Despite that it can handle a variety of functional forms in the Hamiltonian, for instance polynomials in phase space variables, basically also sine and cosine, it cannot be applied to fractional Hamiltonians directly. We summarize the method because it is used to construct the complexifier coherent states in semiclassical perturbation theory in part IV and in its context stability was discussed in [31] in quite a general way. Afterwards we describe in section 19 the so-called algebraic construction of generalized coherent states which is based on the displacement operator construction principle and can be applied to general physical systems as long as their so-called spectrum generating algebra which is often a Lie algebra or a certain Lie subalgebra is known. Since the question arises what exactly spectrum generating algebras used for the algebraic construction are and how one can find them, we discuss this in section 20.

With the aim to find some general stability requirements for algebras, in section 21 we recall the definitions and understanding of stability of semiclassical states we encountered in part V so far and try to combine the most general definition of stability, we encountered, with the algebraic construction principle. To complete this discussion we summarize, compare and discuss some known stability results from the literature [31, 56, 57, 58, 59, 60, 61] and our results concerning stability and its breaking related to algebraic properties.

We combine our findings in sections 22 and 23. We catch up with the idea of an effective Hamiltonian from section 15 in section 22, but this time we apply a so-called Euler rescaling which implies a transformation of the time coordinate. The idea to look for a time transformation was motivated by our consideration about spectrum generating algebras, especially the Kumei method, in section 20. This got us to the point in section 22 that we can extend the phase space and we can express the square root or more general fractional Hamiltonians as constraints on the extended phase space on which they can be reformulated including an alternative, fractional power free Hamiltonian using the Euler Rescaling. Hence, we use in section 22 techniques to construct coherent states for constrained systems. We also catch up with our stability considerations from section 16 and section 17 as well as section 21.

Our findings about generalized annihilation operators throughout part V as well as the algebraic constructions in section 19 inspired us to the proceeding in section 23. There we construct coherent states for square root and more general fractional Hamiltonians which are based on fractional Poisson distributions described in [65, 66]. This construction is adapted to square root or more general fractional Hamiltonians by including a modification of the classical phase space labels that reassembles the fractional powers. The generalized states are also eigenstates of the standard harmonic oscillator annihilation operator. Finally, we sum up and discuss our results in section 24.

Since the detailed conclusions for part III, part IV and part V are distributed over this work, we give an overview and where to find each conclusion as well as an outlook for future research in part VI.

Part II
Review on Loop Quantum Gravity

1 Classical Theory

In this section we will give an introduction to the classical theory of Loop Quantum Gravity (LQG). We start with an introduction to Einstein's equations and derive them from the Einstein-Hilbert action. Next we explain the so-called ADM decomposition which helps us to rewrite the Einstein-Hilbert action in terms of ADM variables, named after Arnowitt, Deser and Misner [14]. Subsequently, the Legendre transformation to come from the Langrangian to the Hamiltonian formulation of gravity is performed. The constraint analysis of this Hamiltonian leads to the gravitational constraints and their algebra, denoted as Dirac or hypersurface deformation algebra. In the last part of this section we introduce the so-called Ashtekar variables to be able to rewrite all variables and constraints into a form close to the form of a Yang-Mills theory. This enables us to quantize the basic variables, constraints and Poisson brackets in the upcoming section.

1.1 Einstein Equations and Einstein-Hilbert Action

We consider the classical equations of motion of General Relativity (GR) in $D+1$ space-time dimensions, that is ***Einstein's equations***, see for example [72, 73, 74, 75],

$$R^{(D+1)}_{\mu\nu}(g) - \frac{1}{2} g_{\mu\nu} R^{(D+1)}(g) = \frac{8\pi G}{c^4} T_{\mu\nu}, \tag{1}$$

where G denotes Newton's constant, c stands for the speed of light, indices run from $\mu, \nu = 0, \ldots, D$ and since we display tensor components here, we implicitly chose a basis, that is a coordinate system. First we will discuss the meaning of the terms on the left and on the right hand side of Einstein's equations. On the left hand side we have the ***space-time metric*** $g_{\mu\nu}$, the ***Ricci tensor*** $R^{(D+1)}_{\mu\nu}$ and the ***Ricci scalar*** $R^{(D+1)}$. The Ricci tensor and the Ricci scalar are both objects derived from the space-time metric $g_{\mu\nu}$ and its derivatives up to second order which is indicated by the argument (g). Mathematically, the metric $g_{\mu\nu}$ is a symmetric non-degenerate tensor field of type $(0, 2)$ on a manifold M. Physically, the metric contains all of the geometrical information about space-time. On the right hand side we have the ***stress-energy-momentum tensor*** $T_{\mu\nu}$, whose components contain all energy-like contributions for matter like photons, fermions,... etc., see for example [74, 75]. The covariant components of the stress-energy-momentum tensor are obtained from the contractions of $T_{\mu\nu}$ with $g^{\mu\nu}$, *i.e.* $T^{\rho\sigma} = g^{\rho\mu} g^{\sigma\nu} T_{\mu\nu}$. The time-time component T^{00} describes the density of relativistic mass, that is the energy density divided by c^2. The time-spatial components $T^{0i} = T^{0i}$, for $i = 1, \ldots, D$ describe the density of the ith component of linear momentum. The spatial-spatial components T^{ik}, $i, k = 1, \ldots, D$, for $i = k$ represent the normal stress, which in case of direction independent systems corresponds to the pressure, and for $i \neq k$ represent the shear stress. So Einstein's equations tell us that geometry and matter interact non-linearly with each other. For example, the accretion of matter, like stars or in the extreme case black holes, bends space-time, which can be observed by the deflection of light from stars behind these objects. This effect was used by Eddington as a first test of GR [76]. The Ricci tensor $R^{(D+1)}_{\mu\nu}$ and the Ricci scalar $R^{(D+1)}$

are contractions of the ***Riemann tensor*** $R^{(D+1)}_{\mu\nu\rho\sigma}$ with the space-time metric $g_{\mu\nu}$ defined by

$$\begin{aligned} R^{(D+1)\sigma}_{\mu\nu\rho} &= \frac{\partial}{\partial x^\nu}\Gamma^\sigma_{\mu\rho} - \frac{\partial}{\partial x^\mu}\Gamma^\sigma_{\nu\rho} + \Gamma^\lambda_{\rho\mu}\Gamma^\sigma_{\nu\lambda} - \Gamma^\lambda_{\rho\nu}\Gamma^\sigma_{\mu\lambda}, \\ R^{(D+1)}_{\mu\nu} &= R^{(D+1)\rho}_{\mu\rho\nu}, \\ R^{(D+1)} &= R^{(D+1)}_{\mu\nu} g^{\mu\nu}, \end{aligned} \tag{2}$$

where we introduced the ***Christoffel symbol*** $\Gamma^\mu_{\nu\rho} := \frac{1}{2} g^{\mu\sigma}\left[\frac{\partial}{\partial x^\rho} g_{\sigma\nu} + \frac{\partial}{\partial x^\nu} g_{\sigma\rho} - \frac{\partial}{\partial x^\sigma} g_{\nu\rho}\right]$. The Christoffel symbol enables us to define a covariant derivative for tensors in GR, the so-called ***Levi-Civita connection*** ∇_μ which is the unique, torsion free and metric compatible connection with respect to $g_{\mu\nu}$. By ***torsion free*** we mean that for a smooth function f from a manifold M into $\mathbb{R}$ we have $(\nabla_\mu\nabla_\nu - \nabla_\nu\nabla_\mu) f = 0$ and for ***metric compatibility*** we demand that $\nabla_\rho g_{\mu\nu} = 0$.

With these definitions in mind, we want to show that Einstein's equations can be derived by the variation of the ***Einstein-Hilbert action***

$$S_{\mathrm{EH}} = \int\limits_M \mathrm{d}^{D+1}Y \sqrt{|\det(g_{\mu\nu})|}\left[\frac{1}{\kappa} R^{(D+1)}(g) + \mathcal{L}_{\mathrm{M}}\right] \tag{3}$$

with $\kappa := \frac{16\pi G}{c^4}$ and $\mathcal{L}_{\mathrm{M}}$ stands for some matter Lagrangian density that gives rise to the stress-energy-momentum tensor $T_{\mu\nu}$. Our presentation of the derivation of Einstein's equations will closely follow the one given in [75]. We choose a coordinate system in which $g_{\mu\nu}$ has diagonal form. This is possible, since $g_{\mu\nu}$ is a symmetric tensor field. To shorten the notation we define $g := \det(g_{\mu\nu})$ and $R := R^{(D+1)}$. The variation of the Einstein-Hilbert action with respect to the inverse metric $g^{\mu\nu}$ yields

$$\delta S_{\mathrm{EH}} = \int\limits_M \mathrm{d}^{D+1}Y \left[\frac{1}{\kappa}\frac{\delta\left(\sqrt{|g|}R(g)\right)}{\delta g^{\mu\nu}(Y)} + \frac{\delta\left(\sqrt{|g|}\mathcal{L}_{\mathrm{M}}\right)}{\delta g^{\mu\nu}(Y)}\right]\delta g^{\mu\nu}(Y) = 0, \tag{4}$$

where $\delta S_{\mathrm{EH}} = 0$ holds due to the action principle. To begin with we calculate the variation of the geometric part of the integrand of the Einstein-Hilbert action

$$\delta\left(\sqrt{|g|}R\right) = \left(\delta\sqrt{|g|}\right) R + \sqrt{|g|}\,(\delta R). \tag{5}$$

The variation of the square root of the determinant of $g_{\mu\nu}$ leads to

$$\delta\sqrt{|g|} = \frac{\mathrm{sgn}(g)}{2\sqrt{|g|}}\delta g = \frac{\mathrm{sgn}(g)}{2\sqrt{|g|}}\,\delta\det(g_{\mu\nu}) = \frac{\mathrm{sgn}(g)}{2\sqrt{|g|}} g g^{\mu\nu}\delta g_{\mu\nu} = -\frac{1}{2}\sqrt{|g|} g_{\mu\nu}\delta g^{\mu\nu}, \tag{6}$$

where we used ***Jacobi's formula*** to calculate the variation of the determinant g and $g^{\mu\nu}\delta g_{\mu\nu} = -g_{\mu\nu}\delta g^{\mu\nu}$. Next we need to determine the variation of the Ricci scalar

$$\delta R = (\delta R_{\mu\nu}) g^{\mu\nu} + R_{\mu\nu}\delta g^{\mu\nu} \tag{7}$$

which ends up in first calculating the variation of the Ricci tensor

$$\delta R_{\mu\nu} = \delta R_{\mu\rho\nu}{}^{\rho} = \frac{\partial}{\partial x^\rho}\delta\Gamma^\rho_{\mu\nu} - \frac{\partial}{\partial x^\mu}\delta\Gamma^\rho_{\rho\nu} + \delta\Gamma^\lambda_{\mu\nu}\Gamma^\rho_{\rho\lambda} + \Gamma^\lambda_{\mu\nu}\delta\Gamma^\rho_{\rho\lambda} - \delta\Gamma^\lambda_{\nu\rho}\Gamma^\rho_{\mu\lambda} - \Gamma^\lambda_{\nu\rho}\delta\Gamma^\rho_{\mu\lambda}. \tag{8}$$

Notice that the Christoffel symbol $\Gamma^{\rho}_{\mu\nu}$ is not a tensor, since its components transform, as shown in [75], as

$$\Gamma^{\nu'}_{\mu'\lambda'} = \frac{\partial x^{\mu}}{\partial x^{\mu'}} \frac{\partial x^{\lambda}}{\partial x^{\lambda'}} \frac{\partial x^{\nu'}}{\partial x^{\nu}} \Gamma^{\nu}_{\mu\lambda} + \frac{\partial x^{\nu'}}{\partial x^{\lambda}} \frac{\partial^2 x^{\lambda}}{\partial x^{\mu'} \partial x^{\lambda'}}, \tag{9}$$

where the second term is contrary to the transformation law for tensor components. Its variation $\delta\Gamma^{\rho}_{\mu\nu}$ is a tensor. From $\nabla_{\rho} g_{\mu\nu} = 0$ one can derive that is equal to

$$\delta\Gamma^{\rho}_{\mu\nu} = \frac{1}{2} g^{\rho\lambda} \left(\nabla_{\mu} \delta g_{\lambda\nu} + \nabla_{\nu} \delta g_{\lambda\mu} - \nabla_{\lambda} \delta g_{\mu\nu} \right) \tag{10}$$

which is a sum of tensors, so $\delta\Gamma^{\rho}_{\mu\nu}$ is a tensor as well. The calculation of the covariant derivative of $\delta\Gamma^{\rho}_{\mu\nu}$ results in

$$\nabla_{\sigma} \left(\delta\Gamma^{\rho}_{\mu\nu} \right) = \frac{\partial}{\partial x^{\sigma}} \left(\delta\Gamma^{\rho}_{\mu\nu} \right) + \Gamma^{\rho}_{\sigma\lambda} \delta\Gamma^{\lambda}_{\mu\nu} - \Gamma^{\lambda}_{\sigma\mu} \delta\Gamma^{\rho}_{\lambda\nu} - \Gamma^{\lambda}_{\sigma\nu} \delta\Gamma^{\rho}_{\lambda\mu}. \tag{11}$$

Inserting this into eq. (8) we obtain the so-called ***Palatini identity***

$$\delta R_{\mu\nu} = \delta R_{\mu\rho\nu}{}^{\rho} = \nabla_{\rho} \left(\delta\Gamma^{\rho}_{\mu\nu} \right) - \nabla_{\nu} \left(\delta\Gamma^{\rho}_{\rho\mu} \right). \tag{12}$$

With this the variation of the Ricci scalar can be written as

$$\delta R = \nabla_{\rho} \left(g^{\mu\nu} \delta\Gamma^{\rho}_{\mu\nu} - g^{\mu\rho} \delta\Gamma^{\lambda}_{\lambda\mu} \right) + R_{\mu\nu} \delta g^{\mu\nu}. \tag{13}$$

It is possible to define the stress-energy-momentum tensor as the variation of the matter Lagrangian density $\mathcal{L}_{\mathrm{M}}$ times a prefactor by

$$T_{\mu\nu} := \frac{-2}{\sqrt{|g|}} \frac{\delta \left(\sqrt{|g|} \mathcal{L}_{\mathrm{M}} \right)}{\delta g^{\mu\nu}}. \tag{14}$$

We insert all of the previous results back into eq. (4) to obtain

$$\begin{aligned} \delta S_{\mathrm{EH}} &= \int\limits_M \mathrm{d}^{D+1} Y \left[\frac{1}{\kappa} \frac{\delta\sqrt{|g|} R}{\delta g^{\mu\nu}} + \frac{1}{\kappa} \frac{\sqrt{|g|} \delta R}{\delta g^{\mu\nu}} - \frac{\sqrt{|g|}}{2} T_{\mu\nu} \right] \delta g^{\mu\nu} \\ &= \int\limits_M \mathrm{d}^{D+1} Y \left[-\frac{\sqrt{|g|}}{2\kappa} g_{\mu\nu} R + \frac{\sqrt{|g|}}{\kappa} \frac{\nabla_{\rho} \left(g^{\mu\nu} \Gamma^{\rho}_{\mu\nu} - g^{\mu\rho} \Gamma^{\lambda}_{\lambda\mu} \right) + R_{\mu\nu} \delta g^{\mu\nu}}{\delta g^{\mu\nu}} - \frac{\sqrt{|g|}}{2} T_{\mu\nu} \right] \delta g^{\mu\nu} \\ &= \int\limits_M \mathrm{d}^{D+1} Y \left[-\frac{1}{2\kappa} g_{\mu\nu} R + \frac{1}{\kappa} R_{\mu\nu} - \frac{1}{2} T_{\mu\nu} \right] \sqrt{|g|} \delta g^{\mu\nu} = 0 \end{aligned} \tag{15}$$

which indeed reproduces Einstein's equations. It was used that in the variation of S_{EH} the term $\sqrt{|g|} \nabla_{\rho} B^{\rho} := \sqrt{|g|} \nabla_{\rho} \left(g^{\mu\nu} \Gamma^{\rho}_{\mu\nu} - g^{\mu\rho} \Gamma^{\lambda}_{\lambda\mu} \right)$ which is equal to $\sqrt{|g|} \nabla_{\rho} B^{\rho} = \partial_{\rho} \left(\sqrt{|g|} B^{\rho} \right)$, since $\sqrt{|g|}$ is a scalar density of weight one, vanishes. This only works, if $\delta g^{\mu\nu}$ vanishes on the boundary or when there is no boundary which is the case for closed, i.e. compact and without a boundary, manifolds M. If the manifold has a boundary, we will have to add the so-called ***Gibbson-Hawking-York boundary term***, for details see [77, 78, 79].

1.2 3+1-ADM Decomposition

In this section our presentation follows the one given in [9] with additional parts gained from [7, 14, 72, 74, 80]. We start with the Einstein-Hilbert action

$$S_{\mathrm{EH}} = \frac{1}{\kappa} \int\limits_M \mathrm{d}^{D+1}Y \sqrt{|\det(g_{\mu\nu})|} R^{(D+1)}(g) \tag{16}$$

in $(D+1)$ dimensions, that is indices run from $\mu, \nu = 0, \ldots, D$. In order to obtain a predictive theory we will see that we need to consider so-called ***globally hyperbolic space-times*** (M, g). ***Predictive*** means that for given initial data on some field ϕ the field equations for ϕ should result in a unique solution and moreover the dependence of the solution on its initial data should be at least continuous and at least locally causal. ***Local causality*** means that the solution is not influenced by a change of initial conditions in space-time regions which are causally not connected. The initial data is given by the knowledge of the field configuration $\phi(t, x)$ and its "velocity" $\dot{\phi}(t, x)$, where we shortly write x for $x^a, a = 1, \ldots, D$, at some instant of time t. In order to have a unique solution, given initial data $\phi(t, x)$ and $\dot{\phi}(t, x)$ at t, it must be possible to compute the solution everywhere on M. Let M be a $(D+1)$ dimensional manifold with a hypersurface denoted here as Σ. An instant of time is a submanifold of M of co-dimension one. So the hypersurface must be a D dimensional spatial manifold. For a general manifold M we might need to take boundary terms into account when we consider an action functional later on, unless we assume that the manifold M is not compact without boundary. We want the hypersurface Σ to be such that every ***causal curve***, meaning its tangent is nowhere spatial, intersects Σ in precisely one point which for example excludes closed causal curves like worm holes. A hypersurface with these properties is called a ***Cauchy surface*** and one says that (M, g) is ***globally hyperbolic***.

According to a theorem by Geroch for homeomorphic maps [81] and later extended by Sanchez and Bernal [82] to diffeomorphic maps between globally hyperbolic space-times and a product space containing a spacelike Cauchy surface of them, we are in the following situation: A globally hyperbolic manifold M is diffeomorphic to $\mathbb{R} \times \sigma$, where σ is any spacelike D dimensional Cauchy surface of M of arbitrary topology. Therefore, we have a ***diffeomorphism***, that is a smooth map

$$\varphi : \mathbb{R} \times \sigma \to M; \quad (\tilde{t}, p) \mapsto X = \varphi(\tilde{t}, p), \tag{17}$$

with smooth inverse

$$\varphi^{-1} : M \to \mathbb{R} \times \sigma; \quad X \mapsto (\tau(X), \gamma(X)), \tag{18}$$

for $\tilde{t} \in \mathbb{R}$, $p \in \sigma$, $X \in M$, smooth diffeomorphisms $\tau : M \to \mathbb{R}$ and $\gamma : M \to \sigma$. We remark that in the article [82] they first proof the existence of the map $M \to \mathbb{R} \times \sigma$ for C^n-spacetimes M, $n \in \mathbb{N}_0$, admitting C^n-Cauchy surfaces which gives rise to C^n-diffeomorphisms φ, τ and γ and then extend these results to the smooth case. If we require a Lorentzian signature for the metric $g_{\mu\nu}$ and have the topology of $\mathbb{R} \times \sigma$, local causality and predictiveness will be ensured.

By means of the diffeomorphism in eq. (17) one can introduce a foliation of the manifold M into spatial hypersurfaces $\Sigma_{\tilde{t}} = \{\tau(X) = \tilde{t}; X \in M\} = \{\varphi(\tilde{t}, p); p \in \sigma\}$, i.e. they have a timelike normal. Now we choose a coordinate system for M or respectively $\mathbb{R} \times \sigma$ and define the $D+1$

vector fields:

$$T(Y) := \frac{\partial \varphi}{\partial t}(t,x)|_{\varphi(t,x)=Y}, \tag{19}$$

$$S_a(Y) := \frac{\partial \varphi}{\partial x^a}(t,x)|_{\varphi(t,x)=Y}, \tag{20}$$

where $Y = Y^\mu$ are the space-time coordinates of M, $\mu, \nu, \rho, \ldots \in \{0, \ldots, D\}$ and $x = x^a$ are the spatial coordinates of σ, $a, b, c, \ldots \in \{1, \ldots, D\}$ and t is the time coordinate.

Let n^μ be the unit timelike normal of the spatial hypersurfaces Σ_t, $t \in \mathbb{R}$, that is $g_{\mu\nu} n^\mu n^\nu = -1$ with $g_{\mu\nu} = g_{\mu\nu}(Y)$ and $n^\mu = n^\mu(Y)$. The S_a are tangent vector fields, i.e. $g_{\mu\nu} S^\mu_a n^\nu = 0$. Using this, we can split the vector field T into its normal and tangential components

$$T^\mu = N n^\mu + N^a S^\mu_a, \tag{21}$$

where we have introduced the so-called ***lapse function*** $N(Y)$ and ***shift vector*** $N^a(Y)$. Now we can select one of the spatial hypersurfaces $\Sigma := \Sigma_{t_0}$ for a fixed but arbitrary t_0 and choose some initial values on Σ. Despite the fact that we choose one fixed Σ, the diffeomorphism invariance of GR in the ADM decomposition is ensured by the point that our choice is completely arbitrary which is encoded in the fact that we do not fix the lapse function $N(Y)$ and the shift vector $N^a(Y)$. We will discuss this in more detail in section 1.3.1 after eq. (83). In what follows we will learn how our fixed but arbitrary choice of Σ leads to a notion of "space" and "time" in the ADM frame.

Definition [9]: Intrinsic Metric and Extrinsic Curvature 1.2.1. *Let ∇_ρ be the unique, torsion free, $g_{\mu\nu}$ compatible, covariant differential induced by $g_{\mu\nu}$, then we define the* ***intrinsic metric*** *$q_{\mu\nu}$ on Σ, the so-called* ***ADM metric****, by*

$$q_{\mu\nu} := g_{\mu\nu} - s n_\mu n_\nu \tag{22}$$

and the ***extrinsic curvature*** *$K_{\mu\nu}$ on Σ by*

$$K_{\mu\nu} := q_\mu{}^\rho q_\nu{}^\sigma \nabla_\rho n_\sigma, \tag{23}$$

where the intrinsic metric $q_{\mu\nu}$ is the spatial part of the space-time metric $g_{\mu\nu}$ with signature s with $s = +1$ in the Euclidean and $s = -1$ in the Lorentzian case.

We will mainly be concerned with the Lorentzian case for causality arguments. The extrinsic curvature $K_{\mu\nu}$ is the spatial projection of the parallel transport of the co-normal n_μ onto Σ, it therefore knows about properties extrinsic to Σ as we observe how n_μ is parallel transported along Σ.

We can pull back all quantities living on M to quantities living on $\Sigma = \varphi_{t=t_0}(\sigma)$ which means that after having chosen a coordinate system, we transform the components of the space-time tensors in the coordinates Y^μ to the components in the coordinates x^a, t and fix $t = t_0$. For the intrinsic metric this gives

$$\begin{aligned} q_{ab}(t,x)|_{t=t_0} &= (\varphi^* q)_{ab}\,(t = t_0, x) \\ &= \frac{\partial \varphi^\mu}{\partial x^a}(t,x) \frac{\partial \varphi^\nu}{\partial x^b}(t,x) q_{\mu\nu}(\varphi(t,x))\,|_{t=t_0} \\ &= (S^\mu_a S^\nu_b q_{\mu\nu})\,(Y)|_{Y=\varphi(t=t_0,x)} \\ &= (S^\mu_a S^\nu_b g_{\mu\nu})\,(Y)|_{Y=\varphi(t=t_0,x)}, \end{aligned} \tag{24}$$

since $S^\mu_a n_\mu = 0$ and analogous for the extrinsic curvature

$$K_{ab}(t,x)|_{t=t_0} = (\varphi^* K)_{ab}(t=t_0,x) \\ = (S^\mu_a S^\nu_b K_{\mu\nu})(Y)|_{Y=\varphi(t=t_0,x)}. \tag{25}$$

We determine the expression for $\sqrt{|\det(g_{\mu\nu})|}$ in the ADM frame. After performing the pull-back to the coordinates x^a and t, the line element $\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}Y^\mu \mathrm{d}Y^\nu$ has the form

$$\mathrm{d}s^2 = g_{tt}\mathrm{d}t^2 + 2g_{at}\mathrm{d}t\mathrm{d}x^a + g_{ab}\mathrm{d}x^a\mathrm{d}x^b. \tag{26}$$

From the definition of the space-time metric $g_{\mu\nu}$ in terms of the intrinsic metric $q_{\mu\nu}$ and the timelike co-normal n_μ to the spatial hypersurface Σ, i.e. $g_{\mu\nu} = q_{\mu\nu} - n_\mu n_\nu$ for $s=-1$, we can read off the components

$$g_{tt} = -N^2 + q_{ab}N^a N^b, \quad g_{ta} = q_{ab}N^b, \quad g_{ab} = q_{ab} \tag{27}$$

and the determinant of the pull-back of the space-time metric $g_{\mu\nu}$ becomes

$$\det(\varphi^* g) = -N^2 \det(q_{ab}). \tag{28}$$

Next we need to express the space-time Ricci scalar $R^{(D+1)} = g^{\mu\rho}g^{\nu\sigma}R^{(D+1)}_{\mu\nu\rho\sigma}$ in terms of the spatial quantities $q_{\mu\nu}$, $K_{\mu\nu}$ and their derivatives, i.e. the spatial Ricci scalar $R^{(D)} = g^{\mu\rho}g^{\nu\sigma}R^{(D)}_{\mu\nu\rho\sigma}$. For this purpose, we remark that the unique, torsion free, $q_{\mu\nu}$ compatible covariant differential D_ρ can be obtained from the unique, torsion free, $g_{\mu\nu}$ compatible covariant differential ∇_ρ by

$$D_\rho T^{\mu_1\ldots\mu_K}_{\nu_1\ldots\nu_J} = q^{\rho'}_\rho \prod_{k=1}^{K} q^{\mu_k}_{\mu'_k} \prod_{j=1}^{J} q^{\nu'_j}_{\nu_j} \left(\nabla_{\rho'} T^{\mu'_1\ldots\mu'_K}_{\nu'_1\ldots\nu'_J}\right), \tag{29}$$

where $T^{\mu_1\ldots\mu_K}_{\nu_1\ldots\nu_J}$ is a spatial tensor on Σ. Notice that for any space-time one form ω_ρ the space-time Riemann tensor $R^{(D+1)}_{\mu\nu\rho\sigma}$ and spatial Riemann tensor $R^{(D)}_{\mu\nu\rho\sigma}$ can be defined by, see for example [74],

$$[\nabla_\mu, \nabla_\nu]\,\omega_\rho =: R^{(D+1)\sigma}_{\mu\nu\rho}\omega_\sigma, \\ [D_\mu, D_\nu]\,\omega_\rho =: R^{(D)\ \sigma}_{\mu\nu\rho}\omega_\sigma. \tag{30}$$

Using these definitions we can derive the so-called ***Gauß equation***, see [9, 80],

$$R^{(D)\ \sigma}_{\mu\nu\rho} = -2K_\rho\,[_\mu K_\nu]^\sigma + q_\mu^{\ \mu'} q_\nu^{\ \nu'} q_\rho^{\ \rho'} q_{\sigma'}^{\ \sigma} R^{(D+1)\sigma'}_{\mu'\nu'\rho'} \tag{31}$$

with this the Ricci scalar of spatial geometry $R^{(D)} = R^{(D)\ \sigma}_{\mu\nu\rho} q_\sigma^{\ \nu} q^{\mu\rho}$ becomes

$$R^{(D)} = -K^2 + K_{\mu\nu}K^{\mu\nu} + q^{\mu\rho}q^{\nu\sigma}R^{(D+1)}_{\mu\nu\rho\sigma}. \tag{32}$$

However, what we want is an expression for $R^{(D+1)} = g^{\mu\rho}g^{\nu\sigma}R^{(D+1)}_{\mu\nu\rho\sigma}$ and not for $q^{\mu\rho}q^{\nu\sigma}R^{(D+1)}_{\mu\nu\rho\sigma}$. This can easily be achieved by using the definition of $q_{\mu\nu}$ and making the replacement $q^{\mu\nu} = g^{\mu\nu} + n^\mu n^\nu$. We obtain

$$q^{\mu\rho}q^{\nu\sigma}R^{(D+1)}_{\mu\nu\rho\sigma} = R^{(D+1)} + g^{\mu\rho}n^\nu\,[\nabla_\mu, \nabla_\nu]\,n_\rho - g^{\nu\sigma}n^\mu\,[\nabla_\mu, \nabla_\nu]\,n_\sigma. \tag{33}$$

To get rid off the second derivative of n_μ we use the definition of the extrinsic curvature $K_{\mu\nu}$ and arrive at the so-called ***Codacci equation***, see [9, 80],

$$R^{(D+1)} = R^{(D)} - K^2 + K_{\mu\nu}K^{\mu\nu} - 2\nabla_\mu v^\mu, \tag{34}$$

where $v^\mu := \nabla_n n^\mu - n^\mu \nabla_\nu n^\nu$ which gives exactly the connection between the spatial and the space-time quantities we wanted to arrive at. The pull-back of $R^{(D)}(Y)$ to Σ yields

$$\begin{aligned} R^{(D)}(t,x)|_{t=t_0} &= \left(\varphi^*\left(R^{(D)}_{\mu\nu\rho\sigma}q^{\mu\rho}q^{\nu\sigma}\right)\right)(t=t_0,x) \\ &= \left(S^\mu_a S^\nu_b S^\rho_c S^\sigma_d R^{(D)}_{\mu\nu\rho\sigma}\right)(Y)|_{Y=\varphi(t=t_0,x)} q^{ac}(t,x)|_{t=t_0} q^{bd}(t,x)|_{t=t_0}, \end{aligned} \tag{35}$$

here we abuse the notation and use the same symbol for $R^{(D)}$ on M and its pull-back on Σ. Moreover, the pull-back of the covariant differential D_μ acting on a one form ω_ν reads

$$\begin{aligned} \left(D_a u_b\right)(t,x)|_{t=t_0} &= \left(\varphi^*\left(D_\mu \omega_\nu\right)\right)(t=t_0,x) \\ &= \left(S^\mu_a S^\nu_b\left(\nabla_\mu \omega_\nu\right)\right)(Y)|_{Y=\varphi(t=t_0,x)} \\ &= \left(\partial_a \omega_u\right)(t,x) - \Gamma^{(D)}_{cab}(t,x)\omega^c(t,x). \end{aligned} \tag{36}$$

Finally, after performing the ADM decomposition and the pull-back to the spatial manifold σ the Einstein-Hilbert action is given by

$$\begin{aligned} S_{\mathrm{EH}} &= \frac{1}{\kappa}\int\limits_M \mathrm{d}^{D+1}Y\,\sqrt{|\det(g_{\mu\nu})|}R^{(D+1)}(Y) \\ &= \frac{1}{\kappa}\int\limits_{\mathbb{R}}\mathrm{d}t\int\limits_\sigma \mathrm{d}^D x\,N\sqrt{\det(q_{ab})}\left(\varphi^* R^{(D)} + K_{ab}K^{ab} - K^2 - \underbrace{2\varphi^*\nabla_\mu v^\mu}_{0}\right)(t,x)|_{t=t_0} \\ &= \frac{1}{\kappa}\int\limits_{\mathbb{R}}\mathrm{d}t\int\limits_\sigma \mathrm{d}^D x\,N\sqrt{\det(q_{ab})}\left(R^{(D)} + K_{ab}K^{ab} - K^2\right)(t,x)|_{t=t_0}. \end{aligned} \tag{37}$$

1.3 Legendre Transformation

The ADM decomposition of the quantities occurring in the Einstein-Hilbert action leads to the expression

$$S_{\mathrm{EH}} = \frac{1}{\kappa}\int\limits_{\mathbb{R}}\mathrm{d}t\int\limits_\sigma \mathrm{d}^D x\,N\sqrt{\det(q_{ab})}\left(R^{(D)}(q) + K_{ab}K^{ab} - K^2\right)(t,x)|_{t=t_0}. \tag{38}$$

Now we want to perform the Legendre transformation in order to rewrite the action in canonical form, i.e. we go over from the Lagrangian to the Hamiltonian formulation. Therefore, let us calculate the canonically conjugate momenta to the configuration variables N, N^a and q_{ab}:

$$\Pi(x) := \frac{\delta^{(D+1)}}{\delta \dot{N}(x)} S_{\mathrm{EH}} = 0, \tag{39}$$

$$\Pi_a(x) := \frac{\delta^{(D+1)}}{\delta \dot{N}^a(x)} S_{\mathrm{EH}} = 0, \tag{40}$$

$$\begin{aligned} p^{ab}(x) := \frac{\delta^{(D+1)}}{\delta \dot{q}_{ab}(x)} S_{\mathrm{EH}} &= \frac{1}{\kappa} N\sqrt{q}\frac{\delta^{(D+1)}}{\delta \dot{q}_{ab}} q^{cd}q^{ef}\left(K_{ce}K_{df} - K_{cd}K_{ef}\right)(x) \\ &= \frac{1}{\kappa}\sqrt{q}\left(K^{ab} - Kq^{ab}\right)(x). \end{aligned} \tag{41}$$

For convenience we define $q := \det(q_{ab})$, $\dot{q}_{ab} := \partial_t q_{ab}$, $\dot{N} := \partial_t N$ and $\dot{N}^a := \partial_t N^a$. In the last equality we used that $\frac{\delta^{(D+1)}}{\delta(\partial_t q_{ab})} K_{cd} = \frac{\delta^{(D+1)}}{\delta(\dot{q}_{ab})} \frac{1}{2N} \left(\dot{q}_{cd} - \left(\pounds_{\vec{N}} q \right)_{cd} \right) = \frac{1}{4N} \left(\delta^a_c \delta^b_d + \delta^a_d \delta^b_c \right)$ and that both q_{ab} and K_{ab} are symmetric as can easily be seen from the definitions of the intrinsic metric and the extrinsic curvature. Here $\pounds_{\vec{N}}$ denotes the ***Lie derivative*** with respect to a vector field $\vec{N}$, for a definition see the appendix A. Notice that the conjugate momenta Π, Π_a to the velocities $\dot{N}$, $\dot{N}^a$ of the lapse function N and the shift vector N^a vanish, which means that Π and Π_a are primary constraints.

We want to rewrite the term $K_{ab}K^{ab} - K^2$ in the Lagrangian density in eq. (38). To achieve this, we reexpress K^{ab} and K in terms of q_{ab} and p^{ab}. We begin with taking the trace of p^{ab} which gives

$$p = q_{ab} p^{ab} = -\frac{D-1}{\kappa} \sqrt{q} K \tag{42}$$

and with $K = -\frac{\kappa}{\sqrt{q}} \frac{p}{(D-1)}$ and the expression for p^{ab} we conclude that

$$K^{ab} = \frac{\kappa}{\sqrt{q}} \left(p^{ab} - q^{ab} \frac{p}{D-1} \right). \tag{43}$$

By inserting the relation between K^{ab} and p^{ab} from eq. (43), we finally arrive at

$$K_{ab}K^{ab} - K^2 = \frac{\kappa^2}{q} \left(p_{ab} p^{ab} - \frac{1}{D-1} p^2 \right). \tag{44}$$

After performing the Legendre transformation the general form of the Hamiltonian becomes

$$\begin{aligned} & H(q_{ab}, p^{ab}, N, N^a, \Pi, \Pi_a) \\ & = \text{extrem}_v \int_\sigma \mathrm{d}^D x \left[\Pi\nu + \Pi_a \nu^a + p^{ab} v_{ab} - \mathcal{L}\Big(q_{ab}, N, N^a, \dot{q}_{ab}, \dot{N}, \dot{N}^a, v_{ab}, \nu, \nu^a \Big) \right](x), \end{aligned} \tag{45}$$

where we extremize with respect to the velocities ν, ν^a, v_{ab} corresponding to the momenta Π, Π_a, p^{ab} denoted by extrem_v and $\mathcal{L}\Big(q_{ab}, N, N^a, \dot{q}_{ab}, \dot{N}, \dot{N}^a, v_{ab}, \nu, \nu^a \Big)$ is the Lagrangian density.

Next we reexpress the term $p^{ab} v_{ab}$ in terms of p^{ab} and q_{ab}. For this purpose, we use the identity $v_{ab} = \dot{q}_{ab} = 2NK_{ab} + \pounds_{\vec{N}} q_{ab}$ to obtain

$$p^{ab} v_{ab} = 2N \frac{\kappa}{\sqrt{q}} \left(p_{ab} p^{ab} - \frac{1}{D-1} p^2 \right) + p^{ab} \pounds_{\vec{N}} q_{ab}. \tag{46}$$

Combining and reinserting eq. (44) and eq. (46) into the Hamiltonian, where we read off the Lagrangian density from eq. (38), leads to

$$\begin{aligned} & H(q_{ab}, p^{ab}, N, N^a, \Pi, \Pi_a)(x) \\ & = \int_\sigma \mathrm{d}^D x \left[\Pi\nu + \Pi_a \nu^a + p^{ab} \left(\pounds_{\vec{N}} q_{ab} \right) + N \left(\frac{\kappa}{\sqrt{q}} \left(p_{ab} p^{ab} - \frac{1}{D-1} p^2 \right) - \frac{\sqrt{q}}{\kappa} R^{(D)}(q) \right) \right](x). \end{aligned} \tag{47}$$

The Hamiltonian $H := H(q_{ab}, p^{ab}, N, N^a, \Pi, \Pi_a)$ contains the velocities ν, ν^a, so we can perform the functional derivative of H with respect to ν, ν^a which enforces

$$\frac{\delta^{(D)} H}{\delta\nu(x)} = \Pi(x) = 0, \tag{48}$$

$$\frac{\delta^{(D)} H}{\delta\nu^a(x)} = \Pi_a(x) = 0. \tag{49}$$

As we will see, to recover the equations of motion in the Hamiltonian framework we need to keep the ν, ν^a as Lagrange multipliers .

In order to understand the meaning of the Lagrange multipliers ν and ν_a, to check the stability of the constraints under the primary Hamiltonian H and finally to see the equivalence to Einstein's equations we calculate the Hamiltonian equations of motion. Let s be the parameter for the evolution with respect to the Hamiltonian H. We start with the Hamiltonian equations of motion for the lapse function N and the shift vector N^a which are

$$\frac{\mathrm{d}}{\mathrm{d}s}N(x) = \{H, N(x)\} = \int_\sigma \mathrm{d}^D y\, \frac{\delta^{(D)}H}{\delta\Pi(y)}\frac{\delta^{(D)}N(x)}{\delta N(y)} = \int_\sigma \mathrm{d}^D y\, \frac{\delta^{(D)}H}{\delta\Pi(y)}\delta^{(D)}(x,y) = \nu(x) \tag{50}$$

and analogous

$$\frac{\mathrm{d}}{\mathrm{d}s}N^a = \{H, N^a(x)\} = \nu^a(x). \tag{51}$$

We remember that the lapse function and the shift vector N, N^a are completely arbitrary which has its origin in the arbitrariness of the diffeomorphism between $\mathbb{R}\times\sigma$ and M. This is in correspondence with the fact that the quantities ν, ν^a do not obey any dynamical evolution law determined by the action, so they are completely arbitrary. Despite that we still have to distinguish carefully between ν, ν^a and N, N^a. Here ν, ν^a are Lagrange multipliers while N, N^a are phase space functions.

The primary constraints Π and Π_a have to be zero at all times. We determine their Hamiltonian equations of motion by calculating the Poisson brackets with the primary Hamiltonian H. This results in

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}\Pi(x) &= \{H, \Pi(x)\} = -\frac{\delta^{(D)}H}{\delta N(x)} =: -C(x),\\ \frac{\mathrm{d}}{\mathrm{d}s}\Pi_a(x) &= \{H, \Pi_a(x)\} = -\frac{\delta^{(D)}H}{\delta N^a(x)} =: -C_a(x)\end{aligned} \tag{52}$$

with

$$\begin{aligned}C &= \frac{\kappa}{\sqrt{q}}\left(p_{ab}p^{ab} - \frac{p^2}{D-1}\right) - \frac{\sqrt{q}}{\kappa}R^{(D)},\\ C_a &= p^{bc}q_{bc,a} - 2(p_a^b)_{,b},\end{aligned} \tag{53}$$

where we obtain the expression for C_a above with the help of the definitions for the ***functional and Lie derivative*** $\pounds$, which are displayed in the appendix A. Given these definitions, we can rewrite C_a from eq. (47) as

$$
\begin{aligned}
&\int\limits_\sigma \mathrm{d}^D x\, \frac{\delta^{(D)} H}{\delta N^a(x)} \delta N^a(x) \qquad (54)\\
&= \frac{\mathrm{d}}{\mathrm{d}\lambda} H(q_{ab}, p^{ab}, N, N^a + \lambda \delta N^a, \Pi, \Pi_a)(x)\,|_{\lambda=0}\\
&= \frac{\mathrm{d}}{\mathrm{d}\lambda} \int\limits_\sigma \mathrm{d}^D x\, p^{ab}(x) \left(\pounds_{\vec{N}+\lambda\delta\vec{N}} q\right)_{ab}(x)\,|_{\lambda=0}\\
&= \int\limits_\sigma \mathrm{d}^D x\, p^{ab}(x) \left(\pounds_{\delta\vec{N}} q\right)_{ab}(x) = \int\limits_\sigma \mathrm{d}^D x\, p^{ab} \left(\delta N^c q_{ab,c} + \delta N^c_{,a} q_{bc} + \delta N^c_{,b} q_{ac}\right)\\
&\overset{\text{P.I.}}{=} \int\limits_\sigma \mathrm{d}^D x \left(p^{ab} q_{ab,c} \delta N^c - 2\left(p^{ab} q_{bc}\right)_{,a} \delta N^c\right)\\
&= \int\limits_\sigma \mathrm{d}^D x \left(p^{bc} q_{bc,a} - 2(p^b_a)_{,b}\right) \delta N^a =: \int\limits_\sigma \mathrm{d}^D x\, C_a \delta N^a.
\end{aligned}
$$

We can further rewrite C_a by noticing that p^{ab} is not a tensor but a tensor density of weight $w = 1$. Therefore, it is possible to decompose p^{ab} and thus p^b_a into $p^b_a = \tilde{p}^b_a \sqrt{q}$, where $\sqrt{q} := \sqrt{\det(q_{ab})}$ is the density factor and $\tilde{p}^b_a$ is a ordinary tensor of type (b, a) , i.e. it has density weight zero. Then, we can compute the covariant derivative D_b of p^b_a which gives

$$
\begin{aligned}
D_b p^b_a &= D_b\left(\sqrt{q}\tilde{p}^b_a\right) = \sqrt{q} D_b \tilde{p}^b_a \qquad (55)\\
&= \sqrt{q}\left(\partial_b \tilde{p}^b_a + \Gamma^b_{bc} \tilde{p}^c_a - \Gamma^c_{ba} \tilde{p}^b_c\right)\\
&= (p^b_a)_{,b} - \frac{1}{2} p^{bc} q_{bc,a},
\end{aligned}
$$

where we used that the spatial covariant derivative D_c is metric compatible with q_{ab}, that is $D_c q_{ab} = 0$. Comparison with the first expression for C_a in eq. (53) leads to the result

$$C_a = -2 q_{ac} D_b p^{bc}. \qquad (56)$$

We find that the primary constraints $\Pi = 0$ and $\Pi_a = 0$ are not automatically preserved in time. They are only preserved in case we consider C and C_a as secondary constraints, such that $C = 0$ and $C_a = 0$ holds. So we need to check, whether the secondary constraints are stable under the Hamiltonian H or not.

1.3.1 Constraint Analysis - Hypersurface Deformation Algebra

Since the secondary constraints C and C_a also appear in smeared form in the Hamiltonian H, we define the smeared constraints by

$$
\begin{aligned}
C(f) &:= \int\limits_\sigma \mathrm{d}^D x\, f(x) C(x), \qquad (57)\\
\vec{C}(\vec{f}) &:= \int\limits_\sigma \mathrm{d}^D x\, f^a(x) C_a(x)
\end{aligned}
$$

with smearing functions f and f^a of rapid decrease. Then the Poisson brackets read

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}\vec{C}(\vec{f}) &= \{H,\vec{C}(\vec{f})\} = \{C(N)+\vec{C}(\vec{N}),\vec{C}(\vec{f})\},\\ \frac{\mathrm{d}}{\mathrm{d}s}C(f) &= \{H,C(f)\} = \{C(N)+\vec{C}(\vec{N}),C(f)\}.\end{aligned} \tag{58}$$

So we need to calculate the individual terms

$$\{\vec{C}(\vec{N}),C(f)\},\quad \{\vec{C}(\vec{N}),\vec{C}(\vec{f})\},\quad \{C(N),C(f)\}. \tag{59}$$

Before we calculate the Poisson brackets of the constraint algebra, we read of from the calculation in eq. (54) that $\vec{C}(\vec{N})$ can be expressed as

$$\vec{C}(\vec{N}) = \int_\sigma \mathrm{d}^D x\, p^{ab}\left(\pounds_{\vec{N}}q\right)_{ab}. \tag{60}$$

With this the calculation of the Poisson brackets of $\vec{C}(\vec{N})$ with q_{ab} and p^{ab} gives rise to

$$\{\vec{C}(\vec{N}),q_{ab}(x)\} = \frac{\delta^{(D)}\vec{C}(\vec{N})}{\delta p^{ab}(x)} = \left(\pounds_{\vec{N}}q\right)_{ab}(x), \tag{61}$$

and

$$\{\vec{C}(\vec{N}),p^{ab}(x)\} = -\frac{\delta^{(D)}\vec{C}(\vec{N})}{\delta q^{ab}(x)} = \Big((\partial_c N^c)p^{ab} + N^c p^{ab}_{,c} - 2N^{(a}_{,c}p^{b)c}\Big)(x). \tag{62}$$

Except the $(\partial_c N^c)$ term, this looks almost like the Lie derivative of a two times contravariant symmetric tensor field t^{ab}

$$\pounds_{\vec{N}}t^{ab} = N^c t^{ab}_{,c} - 2N^{(a}_{,c}t^{b)c} \tag{63}$$

with $k^{(a}s^{b)} = \frac{1}{2}\left(k^a s^b + k^b s^a\right)$. However, as mentioned before p^{ab} is a tensor density of weight one and for tensor densities it can be shown that the Lie derivative $\pounds_{\vec{v}}$ along a vector field $\vec{v}$ of a tensor density T with weight w is given by

$$\pounds_{\vec{v}}T = w\, v^c_{,c}T + \pounds'_{\vec{v}}T, \tag{64}$$

where $\pounds'_{\vec{v}}$ acts on T as it was of weight zero. In this sense we have

$$\{\vec{C}(\vec{N}),p^{ab}\} = \left(\pounds_{\vec{N}}p\right)^{ab}. \tag{65}$$

In summary we derived the identities

$$\begin{aligned}\frac{\delta^{(D)}\vec{C}(\vec{N})}{\delta p^{ab}(x)} &= \{\vec{C}(\vec{N}),q_{ab}(x)\} = \left(\pounds_{\vec{N}}q\right)_{ab}(x),\\ -\frac{\delta^{(D)}\vec{C}(\vec{N})}{\delta q_{ab}(x)} &= \{\vec{C}(\vec{N}),p^{ab}(x)\} = \left(\pounds_{\vec{N}}p\right)^{ab}(x).\end{aligned} \tag{66}$$

The identities in eq. (66) together with the definitions of the functional and the Lie derivative, see A.1 and A.2, can be used to calculate $\{\vec{C}(\vec{N}), C(f)\}$:

$$
\begin{aligned}
\{\vec{C}(\vec{N}), C(f)\} &= \int_\sigma \mathrm{d}^D x\, f(x) \{\vec{C}(\vec{N}), C(x)\} \qquad (67)\\
&= \int_\sigma \mathrm{d}^D x\, f(x) \int \mathrm{d}^D y \left[\frac{\delta^{(D)} \vec{C}(\vec{N})}{\delta p^{ab}(y)} \frac{\delta^{(D)} C(x)}{\delta q_{ab}(y)} - \frac{\delta^{(D)} \vec{C}(\vec{N})}{\delta q_{ab}(y)} \frac{\delta^{(D)} C(x)}{\delta p^{ab}(y)} \right]\\
&= \int_\sigma \mathrm{d}^D x\, f(x) \int \mathrm{d}^D y \left[\left(\pounds_{\vec{N}} q\right)_{ab}(y) \frac{\delta^{(D)} C(x)}{\delta q_{ab}(y)} + \left(\pounds_{\vec{N}} p\right)^{ab}(y) \frac{\delta^{(D)} C(x)}{\delta p^{ab}(y)} \right]\\
&\overset{A.1}{=} \int_\sigma \mathrm{d}^D x\, f(x) \frac{\mathrm{d}}{\mathrm{d}\lambda} C\Big(\left(q_{ab} + \lambda \left(\pounds_{\vec{N}} q\right)_{ab}\right)(x), \Big(p^{ab} + \lambda \left(\pounds_{\vec{N}} p\right)^{ab}\Big)(x) \Big)_{|\lambda=0}\\
&= \int_\sigma \mathrm{d}^D x\, f(x) C\Big(\left(\pounds_{\vec{N}} q\right)_{ab}(x), \left(\pounds_{\vec{N}} p\right)^{ab}(x) \Big)\\
&\overset{A.2}{=} \int_\sigma \mathrm{d}^D x\, f(x) \frac{\mathrm{d}}{\mathrm{d}\lambda} C\Big(\Big(\varphi_\lambda^{\vec{N}}\Big)^* q_{ab}(x), \Big(\varphi_\lambda^{\vec{N}}\Big)^* p^{ab}(x) \Big)_{|\lambda=0}\\
&= \int_\sigma \mathrm{d}^D x\, f(x) \frac{\mathrm{d}}{\mathrm{d}\lambda} \Big(\Big(\varphi_\lambda^{\vec{N}}\Big)^* C \Big)(x)_{|\lambda=0}\\
&= \int_\sigma \mathrm{d}^D x\, f(x) \left(\pounds_{\vec{N}} C\right)(x) = \int_\sigma \mathrm{d}^D x\, f(x) \frac{\partial}{\partial x^a} \left(N^a C\right)(x)\\
&\overset{P.I.}{=} - \int_\sigma \mathrm{d}^D x\, \vec{N}[f] C = -C(\vec{N}[f]) = -C(\pounds_{\vec{N}} f),
\end{aligned}
$$

where $\varphi_\lambda^{\vec{N}}$ is the one-parameter family of diffeomorphisms generated by the integral curves of the vector field $\vec{N}$ and we set $\vec{N}[f] := N^a \partial_a f = \pounds_{\vec{N}} f$. In line four we identify $\left(\pounds_{\vec{N}} q\right)_{ab} = \delta q_{ab}$ and $\left(\pounds_{\vec{N}} p\right)^{ab} = \delta p^{ab}$. Remember, we assume here and in the upcoming that the function f is of rapid decrease such that we can neglect appearing boundary terms which arise from partial integration.

Next we calculate the Poisson bracket $\{\vec{C}(\vec{N}), \vec{C}(\vec{f})\}$:

$$\begin{aligned}
\{\vec{C}(\vec{N}), \vec{C}(\vec{f})\} &= \int_\sigma \mathrm{d}^D x \int_\sigma \mathrm{d}^D y \, \{\left(p^{ab}\left(\pounds_{\vec{N}} q\right)_{ab}\right)(x), \left(p^{cd}\left(\pounds_{\vec{f}} q\right)_{cd}\right)(y)\} \\
&= \int_\sigma \mathrm{d}^D x \int_\sigma \mathrm{d}^D y \, \Big[\left(\pounds_{\vec{N}} q\right)_{ab}(x) p^{cd}(y) \{p^{ab}(x), \left(\pounds_{\vec{f}} q\right)_{cd}(y)\} \\
&+ p^{ab}(x)\left(\pounds_{\vec{f}} q\right)_{cd}(y) \{\left(\pounds_{\vec{N}} q\right)_{ab}(x), p^{cd}(y)\}\Big] \\
&\overset{\text{relable}}{=} \int_\sigma \mathrm{d}^D x \int \mathrm{d}^D y \, p^{cd}(y) \left[\left(\pounds_{\vec{N}} q\right)_{ab}(x) \frac{\delta^{(D)}\left(\pounds_{\vec{f}} q\right)_{cd}(y)}{\delta q_{ab}(x)} - \vec{N} \leftrightarrow \vec{f}\right] \\
&\overset{P.I.}{=} \int_\sigma \mathrm{d}^D x \int \mathrm{d}^D y \, \left[\left(\pounds_{\vec{N}} q\right)_{ab}(x)\left(-\frac{\partial}{\partial y^e}\left(f^e p^{ab}\right)(y) + 2 f^{(a}_{,c} p^{b)c}(y)\right) \delta^{(D)}(x,y) - \vec{N} \leftrightarrow \vec{f}\right] \\
&= \int_\sigma \mathrm{d}^D x \, \left[\left(\pounds_{\vec{N}} q\right)_{ab}\left(-\frac{\partial}{\partial x^e}\left(f^e p^{ab}\right) + 2 f^{(a}_{,c} p^{b)c}\right) - \vec{N} \leftrightarrow \vec{f}\right](x) \\
&= -\int_\sigma \mathrm{d}^D x \, \left[\left(\pounds_{\vec{N}} q\right)_{ab}\left(\pounds_{\vec{f}} p\right)^{ab} - \vec{N} \leftrightarrow \vec{f}\right](x) \\
&= -\int_\sigma \mathrm{d}^D x \, \left[\pounds_{\vec{f}}\left(p^{ab}\left(\pounds_{\vec{N}} q\right)_{ab}\right) - p^{ab}\left(\pounds_{\vec{f}}\left(\pounds_{\vec{N}} q\right)_{ab}\right) - \vec{N} \leftrightarrow \vec{f}\right](x) \\
&= \int_\sigma \mathrm{d}^D x \, p^{ab}\left[\left(\pounds_{\vec{f}} \pounds_{\vec{N}} - \pounds_{\vec{N}} \pounds_{\vec{f}}\right) q\right]_{ab}(x) \\
&= \int_\sigma \mathrm{d}^D x \, p^{ab}\left(\pounds_{[\vec{f}, \vec{N}]} q\right)_{ab}(x) = -\vec{C}([\vec{N}, \vec{f}]),
\end{aligned} \tag{68}$$

where we used the Leibniz rule for the Lie derivative and that

$$\begin{aligned}
\frac{\delta\left(\pounds_{\vec{f}} q\right)_{cd}(y)}{\delta q_{ab}(x)} &= \frac{\delta}{\delta q_{ab}(x)}\left[f^e(y) q_{cd,e}(y) + 2 f^e_{,(c}(y) q_{d)e}(y)\right] \\
&= f^e(y) 2 \delta_c^{(a} \delta_d^{b)}\left[\frac{\partial}{\partial y^e} \delta^{(D)}(x,y)\right] + f^e_{,c}(y) \delta^a_d \delta^b_e \, \delta^{(D)}(x,y) + f^e_{,d}(y) \delta^b_d \delta^a_e \, \delta^{(D)}(x,y).
\end{aligned} \tag{69}$$

To compute the last Poisson bracket $\{C(N), C(f)\}$ we display the Hamiltonian constraint as a sum of two parts

$$C(x) = T(x) + V(x) \tag{70}$$

which we will refer to as the kinetic term $T := \frac{\kappa}{\sqrt{q}}\left(p_{ab} p^{ab} - \frac{p^2}{D-1}\right)$ and the potential term

$V := -\frac{\sqrt{q}}{\kappa}R^{(D)}(q)$. Then the Poisson bracket $\{C(N), C(f)\}$ becomes

$$
\begin{aligned}
\{C(N), C(f)\} &= \int\limits_\sigma \mathrm{d}^D x \int\limits_\sigma \mathrm{d}^D y \, N(x) f(y) \{T(x) + V(x), T(y) + V(y)\} \qquad (71)\\
&= \int\limits_\sigma \mathrm{d}^D x \int\limits_\sigma \mathrm{d}^D y \, N(x) f(y) \left[\{T(x), T(y)\} + \{T(x), V(y)\} + \{V(x), T(y)\} + \underbrace{\{V(x), V(y)\}}_{=0 \text{ depends only on } q_{ab}}\right]\\
&= \int\limits_\sigma \mathrm{d}^D x \int\limits_\sigma \mathrm{d}^D y \, N(x) f(y) \left[\underbrace{\{T(x), T(y)\}}_{\text{interchange } x \leftrightarrow y} + \{T(x), V(y)\} + \underbrace{\{V(x), T(y)\}}_{\text{interchange } x \leftrightarrow y}\right]\\
&= \int\limits_\sigma \mathrm{d}^D x \int\limits_\sigma \mathrm{d}^D y \, [N(x) f(y) - N(y) f(x)] \left[\{T(x), V(y)\} + \frac{1}{2}\{T(x), T(y)\}\right]\\
&= \int\limits_\sigma \mathrm{d}^D x \int\limits_\sigma \mathrm{d}^D y \, [N(x) f(y) - N(y) f(x)] \int\limits_\sigma \mathrm{d}^D z \left(\frac{\delta^{(D)} T(x)}{\delta p^{ab}(z)} \frac{\delta^{(D)} V(y)}{\delta q_{ab}(z)}\right),
\end{aligned}
$$

where we employed that the variation $\frac{\delta^{(D)} V}{\delta p^{ab}} = 0$ vanishes and also the term containing $\frac{1}{2}\{T(x), T(y)\}$ vanishes, since it is ***ultra-local***, i.e. $\frac{1}{2}\{T(x), T(y)\}$ is proportional to $\delta^{(D)}(x, y)$. We can simply calculate the variation of T with respect to q_{ab} and p^{ab}, namely

$$
\begin{aligned}
\frac{\delta^{(D)} T(x)}{\delta q_{ab}(z)} &= -\frac{\kappa}{2\sqrt{q}} q^{ab} \left(p_{cd} p^{cd} - \frac{p^2}{D-1}\right) \delta^{(D)}(x, z) \qquad (72)\\
\frac{\delta^{(D)} T(x)}{\delta p^{ab}(z)} &= \frac{2\kappa}{\sqrt{q}} \left(p_{ab} - \frac{p}{D-1} q_{ab}\right) \delta^{(D)}(x, z)\,.
\end{aligned}
$$

This indeed shows that the term containing $\frac{1}{2}\{T(x), T(y)\}$ is going to vanish after performing the integral.

Now the variation of the potential term $V = -\frac{\sqrt{q}}{\kappa}R^{(D)}(q)$ yields

$$
\begin{aligned}
\delta V &= -\frac{1}{\kappa}\delta\left(\sqrt{q} R^{(D)}(q)\right) \qquad (73)\\
&= -\frac{1}{\kappa}\left[\delta\left(\sqrt{q} q^{ab} R^{(D)}_{ab}(q)\right)\right]\\
&= -\frac{1}{\kappa}\left[(\delta\sqrt{q})\, q^{ab} R^{(D)}_{ab}(q) + \sqrt{q}\left(\delta q^{ab}\right) R^{(D)}_{ab}(q) + \sqrt{q} q^{ab}\left(\delta R^{(D)}_{ab}(q)\right)\right]\\
&= -\frac{1}{\kappa}\left[\sqrt{q}\left(\frac{1}{2}R^{(D)} q^{ab} - q^{ca} q^{db} R^{(D)}_{cd}\right)\delta q_{ab} + \sqrt{q} q^{ab}\left(\delta R^{(D)}_{ab}(q)\right)\right]\\
&= -\frac{1}{\kappa}\left[\sqrt{q}\left(\frac{1}{2}R^{(D)} q^{ab} - R^{(D)ab}\right)\delta q_{ab} + \sqrt{q} q^{ac}\left(\delta R^{(D)\ b}_{abc}\right)\right]\\
&= -\frac{1}{\kappa}\left[-\sqrt{q} G^{(D)ab}\delta q_{ab} + \sqrt{q} q^{ac}\left(\delta R^{(D)\ b}_{abc}\right)\right]
\end{aligned}
$$

and we introduced the symbol $G^{(D)ab}$ for the ***Einstein tensor of spatial geometry***. Similar we can define $G^{(D)a0}$ for the spatial-time and $G^{(D)00}$ for the time-time components. In line four we used that $\delta q = \delta \det(q_{ab}) = q q^{ab} \delta q_{ab}$ and $\delta \delta^a_b = \delta\left(q^{ac} q_{cb}\right) = 0$, consequently $\delta\sqrt{q} = \frac{1}{2}\sqrt{q} q^{ab}\delta q_{ab}$ and $\delta q^{cd} = -q^{ca} q^{db} \delta q_{ab}$.

We assume in the following that the constraints and vacuum Einstein's equations are satisfied, that is $G^{(D)ab} = 0$, $G^{(D)a0} = 0$ and $G^{(D)00} = 0$. To calculate the variation of the Ricci tensor $\delta R^{(D)\ b}_{abc}$ we use the definition of the Riemann tensor in terms of the Christoffel symbols $R_{abc}{}^{d} = \partial_b \Gamma^d_{ac} - \partial_a \Gamma^d_{bc} + \Gamma^f_{ca}\Gamma^d_{bf} - \Gamma^f_{cb}\Gamma^d_{af}$. Recall that $\Gamma_{ab}^{\ c}$ is not a tensor, however its variation $\delta\Gamma_{ab}^{\ c}$ is a tensor and we can show using the definition of the covariant derivative D_a, also compare section 1.1, that

$$\begin{aligned}\delta R_{abc}{}^{d} &= D_b \delta\Gamma^d_{ac} - D_a \delta\Gamma^d_{bc} =: -2D_{[a}\delta\Gamma^d_{b]c}, \qquad (74)\\ \delta\Gamma^a_{bc} &= \frac{1}{2} q^{ae} \left(D_c \delta q_{eb} + D_b \delta q_{ec} - D_e \delta q_{bc} \right)\end{aligned}$$

with $D_a \delta q_{bc} \neq 0$ despite that $D_a q_{bc} = 0$. Let $h(y)$ be a test function of rapid decrease, i.e. an element of the Schwarz space. Consider the variation of the integral, where we apply the results from eq. (73) and eq. (74), especially for $G^{(D)ab} = 0$ we have

$$\begin{aligned}
&\int_\sigma \mathrm{d}^D y\, h(y)\, \delta\left(\sqrt{q} R^{(D)}\right)(y) = \int_\sigma \mathrm{d}^D y\, h \sqrt{q} q^{ac} \delta R^{(D)\ b}_{abc} \qquad (75)\\
&= -2 \int_\sigma \mathrm{d}^D y\, h \sqrt{q} q^{ac} D_{[a}\delta\Gamma^b_{b]c} = -2 \int_\sigma \mathrm{d}^D y\, h \sqrt{q} q^{c[a} D_a \delta\Gamma^{b]}_{bc}\\
&\overset{metric\ comp.}{=} -2 \int_\sigma \mathrm{d}^D y\, D_a \left(h \sqrt{q} q^{c[a} \delta\Gamma^{b]}_{bc} \right) + 2 \int_\sigma \mathrm{d}^D y\ (D_a h) \sqrt{q} q^{c[a} \delta\Gamma^{b]}_{bc}\\
&=: B_1(h) + \int_\sigma \mathrm{d}^D y\ (D_a h) \sqrt{q} q^{c[a} q^{b]e} D_c \delta q_{eb}\\
&+ \int_\sigma \mathrm{d}^D y\ (D_a h) \sqrt{q} q^{c[a} q^{b]e} D_b \delta q_{ec} - \int_\sigma \mathrm{d}^D y\ (D_a h) \sqrt{q} q^{c[a} q^{b]e} D_e \delta q_{bc}\\
&= B_1(h) + 2 \int_\sigma \mathrm{d}^D y\ (D_a h) \sqrt{q} q^{c[a} q^{b]e} D_c \delta q_{eb}\\
&= B_1(h) + 2 \int_\sigma \mathrm{d}^D y\, D_c \left((D_a h) \sqrt{q} q^{c[a} q^{b]e} \delta q_{eb} \right) - 2 \int_\sigma \mathrm{d}^D y\ (D_c D_a h) \sqrt{q} q^{c[a} q^{b]e} \delta q_{eb}\\
&=: B_1(h) + B_2(h) - 2 \int_\sigma \mathrm{d}^D y\ (D_c D_a h) \sqrt{q} q^{c[a} q^{b]e} \delta q_{eb}.
\end{aligned}$$

When we take into account that here the covariant derivative D_a of a tensor density of weight one V^a reduces to the partial derivative ∂_a, i.e. $D_a V^a = \partial_a V^a$, since the contributions from the Christoffel symbols cancel against each other, the ***boundary terms*** $B_1(h)$ and $B_2(h)$ read

$$B_1(h) := -2 \int_\sigma \mathrm{d}^D y\, \frac{\partial}{\partial y^a} \left(h \sqrt{q} q^{c[a} \delta\Gamma_{bc}^{\ \ b]} \right)(y), \qquad (76)$$

$$B_2(h) := 2 \int_\sigma \mathrm{d}^D y\, \frac{\partial}{\partial y^c} \left((D_a h) \sqrt{q} q^{a[c} q^{e]b} \delta q_{eb} \right)(y). \qquad (77)$$

The boundary terms can be dropped for smearing functions of rapid decrease which we are supposed to do in the following. Finally, the Poisson bracket becomes

$$\begin{aligned}
\{C(N), C(f)\} &= 4 \int_\sigma \mathrm{d}^D x \left[N \left(p_{ab} - \frac{p}{D-1} q_{ab} \right) q^{a[b} q^{c]d} D_c D_d f - N \leftrightarrow f \right] \\
&= -2 \int \mathrm{d}^D x \left(N p^{ab} D_a D_b f - f p^{ab} D_a D_b N \right) \\
&= -2 \int \mathrm{d}^D x \, D_a \left(N p^{ab} D_b f - f p^{ab} D_b N \right) \\
&+ 2 \int_\sigma \mathrm{d}^D x \left[p^{ab} \left(D_a N \right) \left(D_b f \right) - p^{ab} \left(D_a f \right) \left(D_b N \right) + \left(D_a p^{ab} \right) \left(N D_b f - f D_b N \right) \right] \\
&=: B_3(N, f) + 2 \int_\sigma \mathrm{d}^D x \left(D_a p^{ab} \right) \left(N D_b f - f D_b N \right) \\
&= - \int_\sigma \mathrm{d}^D x \left(-2 q_{ac} D_d p^{dc} \right) q^{ab} \left(N \partial_b f - f \partial_b N \right) \\
&= - \int_\sigma \mathrm{d}^D x \, C_a q^{ab} \left(N \partial_b f - f \partial_b N \right) \\
&=: -\vec{C} \left(\vec{q}^{\,-1} \left(N \mathrm{d} f - f \mathrm{d} N \right) \right) .
\end{aligned} \tag{78}$$

The second and third term vanish due to the symmetry in the derivative of the functions f and N. For functions N and f of rapid decrease we can drop the ***boundary term***

$$B_3(N, f) := -2 \int_\sigma \mathrm{d}^D x \, \frac{\partial}{\partial x^a} \left(N p^{ab} D_b f - f p^{ab} D_b N \right) . \tag{79}$$

We obtain the so-called ***hypersurface deformation algebra***, see [15, 16]:

$$\begin{aligned}
\{\vec{C}(\vec{N}), \vec{C}(\vec{f})\} &= -\vec{C}([\vec{N}, \vec{f}]) = -\vec{C}(\pounds_{\vec{N}} \vec{f}) \\
\{\vec{C}(\vec{N}), C(f)\} &= -C(\vec{N}[f]) = -C(\pounds_{\vec{N}} f) \\
\{C(N), C(f)\} &= -\vec{C} \left(\vec{q}^{\,-1} \left(N \mathrm{d} f - f \mathrm{d} N \right) \right)
\end{aligned} \tag{80}$$

This shows that the constraints are first class constraints and the third Poisson bracket in eq. (80) contains a phase space dependent structure function, for details on the definition of first class constraints see section 4, hence we have no Lie algebra, but a so-called ***Lie algebroid***. Later we will come back to this point.

In summary, the stability analysis of the secondary constraints $C = 0$, $C_a = 0$ arose in the following picture: The evaluation of the Poisson brackets gives us

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}s} \vec{C}(\vec{f}) &= \{H, \vec{C}(\vec{f})\} = - \left[\vec{C}([\vec{N}, \vec{f}]) - C(\vec{f}[N]) \right] , \\
\frac{\mathrm{d}}{\mathrm{d}s} C(N) &= \{H, C(f)\} = - \left[C(\vec{N}[f]) + \vec{C} \left(\vec{q}^{\,-1} \left(N \mathrm{d} f - f \mathrm{d} N \right) \right) \right] .
\end{aligned} \tag{81}$$

So in case the constraints vanish $C(f) = \vec{C}(\vec{f}) = 0$ for all $f, \vec{f}$, consequently also the evolved constraints vanish $\frac{\mathrm{d}}{\mathrm{d}s}C(f) = \frac{\mathrm{d}}{\mathrm{d}s}\vec{C}(\vec{f}) = 0$ for all $f, \vec{f}$. Therefore, the secondary constraints $C = 0$, $C_a = 0$ are stable under evolution with respect to the Hamiltonian H. Notice that we did not write time-evolution here for the reason we are going to explain next.

The Hamiltonian H is a linear combination of primary and secondary constraints given by

$$H = \int \mathrm{d}^D x \, (\nu\Pi + \nu^a\Pi_a + NC + N^a C_a) , \tag{82}$$

with $\Pi = \frac{\delta S_{\mathrm{EH}}}{\delta \dot{N}} = 0$, $\Pi_a = \frac{\delta S_{\mathrm{EH}}}{\delta \dot{N}^a} = 0$ and

$$\frac{\mathrm{d}}{\mathrm{d}s}N = \nu(x), \quad \frac{\mathrm{d}}{\mathrm{d}s}N^a = \nu^a(x), \quad \frac{\mathrm{d}}{\mathrm{d}s}\Pi = -C = 0, \quad \frac{\mathrm{d}}{\mathrm{d}s}\Pi_a = -C_a = 0. \tag{83}$$

Furthermore, we have

$$\frac{\mathrm{d}}{\mathrm{d}s}q_{ab} = \{C(N) + \vec{C}(\vec{N}), q_{ab}\}, \quad \frac{\mathrm{d}}{\mathrm{d}s}p^{ab} = \{C(N) + \vec{C}(\vec{N}), p^{ab}\}. \tag{84}$$

We gained the Lagrange multipliers $\nu(x)$, $\nu^a(x)$ which are completely arbitrary functions and we have the lapse function and shift vector N, N^a which are arbitrary phase space functions. Later on we consider the reduced ADM phase space which means that one sets $\Pi = 0$ and $\Pi^a = 0$. Then N and N^a will become Lagrange multipliers as well. The arbitrariness of the functions can be explained by the interpretation that the Hamiltonian H here does not generate time translations, as we expect from classical theories, it generates gauge transformations with respect to time. So here the parameter s has not a physical meaning.

We can classify the gauge transformations generated by H as follows. Remember that

$$\{\vec{C}(\vec{N}), q_{ab}\} = \left(\pounds_{\vec{N}} q\right)_{ab} , \tag{85}$$

$$\{\vec{C}(\vec{N}), p^{ab}\} = \left(\pounds_{\vec{N}} p\right)^{ab} . \tag{86}$$

These identities tell us that $\vec{C}(\vec{N})$ generates spatial diffeomorphisms of q_{ab} and p^{ab} on Σ along the integral curves of the vector field $\vec{N}$. We are left with the investigation of the action of the remaining constraint $C(N)$ on q_{ab} and p^{ab}. From the constraint stability analysis we got

$$\frac{d}{ds}q_{ab} = \{H, q_{ab}\} = \{C(N), q_{ab}\} + \{\vec{C}(\vec{N}), q_{ab}\} = \{C(N), q_{ab}\} + \left(\pounds_{\vec{N}} q\right)_{ab} , \tag{87}$$

which gives us an expression for $\{C(N), q_{ab}\}$, explicitly

$$\{C(N), q_{ab}\} = \frac{d}{ds}q_{ab} - \left(\pounds_{\vec{N}} q\right)_{ab} . \tag{88}$$

In case we identify the foliation parameter t with the evolution parameter s we can make use of $K_{ab} = \frac{1}{2N}\left(\partial_t q_{ab} - \left(\pounds_{\vec{N}} q\right)_{ab}\right)$ and one can show that $(\pounds_{Nn} q)_{ab} = 2NK_{ab}$. Putting all of this together, we end up with the following expression

$$\{C(N), q_{ab}\} = (\pounds_{Nn} q)_{ab} . \tag{89}$$

The constraint $C(N)$ generates diffeomorphisms of q_{ab} orthogonal to the hypersurface.
We need to check whether this is also true for p^{ab}. Again, we can use our results of the stability analysis and of eq. (85) to obtain

$$\{C(N), p^{ab}\} = \{H - \vec{C}(\vec{N}), p^{ab}\} = \dot{p}^{ab} - \left(\pounds_{\vec{N}} p\right)^{ab} . \tag{90}$$

Here we only mention that it is possible to show that $\dot{p}^{ab} - \left(\pounds_{\vec{N}} p\right)^{ab} = \left(\pounds_{Nn} p\right)^{ab}$ which was calculated in [9, 80]. A straightforward calculation of $\{C(N), p^{ab}\}$ making use of the results in 1.3 gives

$$\begin{aligned}\{C(N), p^{ab}\} = &-\frac{2N\kappa}{\sqrt{q}}\left(p^a_c p^{cb} - p\frac{p^{ab}}{D-1}\right) + \frac{N}{2}q^{ab}C \\ &+ \frac{\sqrt{q}}{\kappa}\left(N\left[q^{ab}R^{(D)} - R^{(D)ab}\right] - 2q^{a[b}q^{c]d}D_c D_d N\right).\end{aligned} \tag{91}$$

This leads us to the question whether this expression is equal to $\left(\pounds_{Nn} p\right)^{ab}$. The equality

$$\begin{aligned}\{C(N), p^{ab}\} &= \left(\pounds_{Nn} p\right)^{ab} \\ &= -\frac{2N\kappa}{\sqrt{q}}\left(p^a_c p^{cb} - p\frac{p^{ab}}{D-1}\right) + \frac{N}{2}q^{ab}C \\ &+ \frac{\sqrt{q}}{\kappa}\left(N\left[q^{ab}R^{(D)} - R^{(D)ab}\right] - 2q^{a[b}q^{c]d}D_c D_d N\right).\end{aligned} \tag{92}$$

is rather confusing because on the one hand we get $\{C(N), p^{ab}\} = \left(\pounds_{Nn} p\right)^{ab}$ which gives rise to the same interpretation for the action of $C(N)$ on p^{ab} as it did for q_{ab} but on the other hand the expression of the second identity does not look at all as $\left(\pounds_{Nn} p\right)^{ab}$. To solve this obstacle one has to lift the quantities from Σ back to the space-time manifold M and use $p^{\mu\nu} = \frac{\sqrt{q}}{\kappa}\left(K^{\mu\nu} - Kq^{\mu\nu}\right)$ as well as $2NK_{\mu\nu} = \left(\pounds_{Nn} q\right)_{\mu\nu}$. After a rather lengthy calculation, for details see [9], one arrives at

$$\begin{aligned}&\{C(N), p^{\mu\nu}\} - \left(\pounds_{Nn} p\right)^{\mu\nu} \\ &= N\frac{\sqrt{q}}{\kappa}\left(q^{\mu\nu}q^{\rho\sigma} - q^{\mu\rho}q^{\nu\sigma}\right)R^{(D+1)}_{\rho\sigma} + \frac{1}{2}Nq^{\mu\nu}C.\end{aligned} \tag{93}$$

The following observation sheds some light on this result. Consider the Einstein tensor of $g_{\mu\nu}$ on M given by $G^{(D+1)}_{\mu\nu} = R^{(D+1)}_{\mu\nu} + \frac{1}{2}g_{\mu\nu}R^{(D+1)}$ and recall from section 1.2 that $q^{\mu\nu} = g^{\mu\nu} - sn^\mu n^\nu$. Then we recover, see [9], the temporal-spatial projection of the Einstein tensor

$$n^\mu n^\nu G^{(D+1)}_{\mu\nu} = \frac{\kappa}{2}\frac{sC}{\sqrt{q}} \tag{94}$$

and the temporal-temporal projection of the Einstein tensor

$$q^\mu_\rho n^\nu G^{(D+1)}_{\mu\nu} = -\frac{\kappa}{2}\frac{sC_\rho}{\sqrt{q}}. \tag{95}$$

The mismatch between $\{C(N), p^{\mu\nu}\}$ and $\left(\pounds_{Nn} p\right)^{\mu\nu}$ can be eliminated by demanding that the equations of motion given by the vacuum Einstein's equations are satisfied, that is $G^{(D+1)}_{\mu\nu} = 0$. Consequently, since for GR we have $\sqrt{q} > 0$, the constraints C and C_ρ need to be satisfied, that is $C = 0$ and $C_\rho = 0$ for all ρ to make the left hand side of the equations vanish.

We conclude: transformations generated by H can be interpreted as space-time diffeomorphisms along the foliation vector field $T = Nn^\mu + N^a\varphi^\mu_{,a}$ in case that

1. We identify the Hamiltonian evolution parameter s with the foliation parameter t.

2. The vacuum Einstein's equations hold, that is $G^{(D+1)}_{\mu\nu} = 0$.

This might be misleading, since the Einstein-Hilbert action $S_{\rm EH}$ is always invariant under the group of (passive) space-time diffeomorphisms, denoted by Diff(M), irrespective of the fact whether the equations of motions hold or not. In contrast, we have the interpretation of the gauge transformations, generated by the Hamiltonian $C(N)$ and diffeomorphism constraint $\vec{C}(\vec{N})$, as infinitesimal space-time diffeomorphisms which only holds if the equations of motion are satisfied. The set of all transformations generated by the Hamiltonian and diffeomorphism constraint is called the ***Bergmann-Komar "group"*** BK(M), see for example [83, 84, 85]. Only on-shell the two groups are equal, i.e. Diff(M) = BK(M) iff $G^{(D+1)}_{\mu\nu} = 0$. Strictly speaking the Bergmann-Komar "group" BK(M) is no group at all because its underlying algebra, which is the hypersurface deformation algebra, is generated by the set of all $C(N)$, $\vec{C}(\vec{N})$ which is no Lie algebra but a ***Lie algebroid*** due to the phase space dependent structure functions q^{-1} in $\{C(N), C(f)\} = -\vec{C}\left(\vec{q}^{\,-1}\left(N{\rm d}f - f{\rm d}N\right)\right)$. On the contrary, the diffeomorphism algebra diff(M) of the space-time diffeomorphism group Diff(M) is a Lie algebra isomorphic to the algebra of vector fields on M. So we will have two actions on our tensor fields on M: first the action of the kinematical group Diff(M) and second the action of the dynamical group BK(M). While the implementation in quantum theory will be different, in the semiclassical limit there should not be any difference, since classically the vacuum Einstein equations hold, for details compare [83, 84, 85].

1.4 Ashtekar Variables

We presented in section 1.2 the formulation of GR in the ADM variables, that is in terms of the intrinsic (spatial) metric q_{ab} and its canonically conjugate momentum p^{ab}. They give rise to a Poisson*-subalgebra $\mathfrak{P}$ of the classical phase space of GR and one can also define an abstract quantum*-algebra $\mathfrak{Q}$ based on the classical Poisson*-subalgebra of the ADM variables. However, until today people were not successful in finding a well defined, background independent representation of $\mathfrak{Q}$ which is also compatible with the formulation of the Hamiltonian constraint operator. For a different set of variables the situation changes. In 1986 Ashtekar, see [86, 87], found new canonical variables which make it possible to cast GR into the form of Yang-Mills gauge theories which are familiar from Quantum Field Theory (QFT). The formulation of GR in the new canonical variables consist of the following steps: the first step consists of an extension of the classical ADM phase space which leads to an additional constraint, known as Gauß constraint. A symplectic reduction (reduction compatible with the symplectic structure) with respect to this new constraint reproduces the ADM quantities and their associated Poisson algebra. An extension of the phase space with the occurrence of new constraints can even be used in more common ways as we will see in chapter III. In the second step we perform a canonical transformation that is a composition of a constant Weyl transformation and an affine transformation, which will be explained in detail below. Our procedure here follows the one given in [9] with supplements from [7, 80].

We start with the definition of a $(D+1)$-***bein*** or ***triad*** in $(D+1)$ dimensions. A $(D+1)$-bein is a $(D+1)$-tuple of co-vectors e^I_μ with internal indices $I = 0, 1, \ldots, D$ and tensorial space-time indices $\mu = 0, 1, \ldots, D$, such that in case an ***internal metric*** η_{IJ} exists a space-time metric $g_{\mu\nu}$ is defined by

$$g_{\mu\nu} := \eta_{IJ} e^I_\mu e^J_\nu. \tag{96}$$

Here we want η_{IJ} to be the ***Minkowski metric***, such that $g_{\mu\nu}$ is also a metric of Lorentz signature $(-1,1,1,1)$. Since the metric $g_{\mu\nu}$ is non-singular, also the $(D+1)$-bein e^I_μ is non-singular and we can define the inverse $(D+1)$-bein e^μ_I by demanding that

$$e^\mu_I e^J_\mu = \delta^J_I, \quad e^\mu_I e^I_\nu = \delta^\mu_\nu \tag{97}$$

with which it is easy to show that $e^\mu_I = g^{\mu\lambda}\eta_{IK}e^K_\lambda$ and $e^J_\nu = g_{\nu\lambda}\eta^{JK}e^\lambda_K$ for $\eta_{IK}\eta^{KJ} = \delta^J_I$. The extension from $g_{\mu\nu}$ to e^I_μ adds additional gauge degrees of freedom to our theory as will become clear when we go over to the ADM framework. Due to representational issues, the comparison with the ADM framework works only in $D+1=4$ dimensions. We are going to discuss these issues in the course of this section. Despite that there exist more complicated higher dimensional generalizations, see for example [88, 89, 90]. Let us write down the components of a space-time metric $g_{\mu\nu}$ after performing the ADM decomposition and in terms of 4-beins which looks like

$$\begin{aligned} g_{tt} &= -N^2 + q_{ab}N^aN^b = -(e^0_t)^2 + \delta_{jk}e^j_te^k_t, \\ g_{ta} &= q_{ab}N^b = -e^0_te^0_a + \delta_{jk}e^j_ae^k_t, \\ g_{ab} &= q_{ab} = -e^0_ae^0_b + \delta_{jk}e^j_ae^k_b. \end{aligned} \tag{98}$$

We count the degrees of freedom (d.o.f.) of the 4-bein: For e^0_t we have 1 d.o.f, each of the elements e^j_t and e^0_a gives us 3 d.o.f. and for the remaining e^j_a we get 9 d.o.f.. Altogether this gives 16 d.o.f. for the 4-bein.

Since the metric $g_{\mu\nu}$ has 10 components, we are left with 6 additional degrees of freedom which correspond to the gauge group of SO$(1,3)$. We can partially fix the SO$(1,3)$ gauge freedom to a SO(3) gauge freedom by imposing the so called ***time gauge*** :

$$e^0_\mu = n_\mu \Rightarrow e^0_a = 0, \tag{99}$$

since in the ADM frame the co-normal n_μ to the hypersurface has components $n_a = 0$ and $n_t = -N$. Then we can solve the 10 equations above to obtain

$$q_{ab} = \delta_{jk}e^j_ae^k_b, \quad e^j_t = e^j_aN^a, \quad e^0_t = -N. \tag{100}$$

The spatial metric q_{ab} in terms of e^j_a is no longer invariant under SO$(1,3)$, but only under SO(3) because δ_{jk} is invariant under local rotations $O \in$ SO(3) that is $\delta_{jk}O^j_m(x)O^k_n(x) = \delta_{mn}$ as well as $e^i_a = O^i_je^j_a$, i.e. the time gauge has frozen the boost part of SO$(1,3)$. Notice that the definition of q_{ab} and the local rotation invariance of $q_{ab} = \delta_{jk}e^j_ae^k_b$ also works in D dimensions, that is for $j,k = 1\dots,D$. For $D=3$ the 3-bein e^i_a can be viewed as an su(2)-valued one form due to so(3) $\cong$ su(2). Now we introduce another one form K^i_a from which we can derive the extrinsic curvature K_{ab} by

$$-sK_{ab} := \frac{1}{2}\left(K^i_ae^j_b\delta_{ij} + K^i_be^j_a\delta_{ij}\right) \tag{101}$$

where $s=-1$ for Lorentzian signature of $g_{\mu\nu}$. Also K^i_a is for $D=3$ an su(2)-valued one form. Since K_{ab} is a symmetric tensor field, the additional condition $G_{ab} := \frac{1}{2}\left(K^i_ae^i_b - K^i_be^i_a\right) = 0$ needs to be satisfied. We introduce the so-called ***densitized triad*** ("electric fields") in D dimensions by

$$E^a_j := \mathrm{sgn}\left(\det\left(e^i_a\right)\right)\frac{1}{(D-1)!}\epsilon^{aa_1\dots a_{D-1}}\epsilon_{jj_1\dots j_{D-1}}e^{j_1}_{a_1}\dots e^{j_{D-1}}_{a_{D-1}} = \sqrt{q}e^a_j. \tag{102}$$

Using this definition instead of $G_{ab}=0$, we can equivalently demand that

$$G_{jk} := \frac{1}{2}\left(K_{aj}E^a_k - K_{ak}E^a_j\right) = 0. \tag{103}$$

The extended phase space coordinatized by $\left(K_a^i, E_i^a\right)$ can be equipped with the following symplectic structure

$$\begin{aligned} \{E_j^a(x), K_b^k(y)\} &= \frac{\kappa}{2}\delta_b^a\delta_j^k\delta^{(3)}(x,y), \\ \{E_j^a(x), E_k^b(y)\} &= \{K_a^j(x), K_b^k(y)\} = 0. \end{aligned} \tag{104}$$

In the next step we want to establish the notion of a ***spin connection***. The spin connection is the extension of the spatial covariant derivative D_a^{old} from ordinary tensors to mixed tensors with tensorial and so(D) indices. It is given by

$$D_a t_{b\ldots j\ldots}^{c\ldots k\ldots} := D_a^{\text{old}} t_{b\ldots j\ldots}^{c\ldots k\ldots} + \Gamma_{aj}^{\ell} t_{b\ldots \ell\ldots}^{c\ldots k\ldots} + \Gamma_{ac}^{k} t_{b\ldots j\ldots}^{c\ldots \ell\ldots}, \tag{105}$$

where $a, b, c, \ldots$ are contracted with q_{ab} and $j, k, \ell, \ldots$ with δ_{jk}.

Then the extension of the q_{ab} metric compatible covariant derivative D_a^{old}, i.e. $D_a^{\text{old}} q_{bc} = 0$, can be defined as the spin connection of the 3-bein e_a^j by

$$D_a e_b^j := \partial_a e_b^j - \Gamma_{ab}^c e_c^j + \Gamma_{ak}^j e_b^k = 0. \tag{106}$$

which allows to express Γ_{ak}^j in terms of the 3-beins and Γ_{ab}^c, namely

$$\Gamma_{ak}^j = \Gamma_{ajk} = -e_k^b \left[\partial_a e_b^j - \Gamma_{ab}^c e_c^j\right]. \tag{107}$$

Often only Γ_{ak}^j is denoted as spin connection. The position of the indices $j, k, \ldots$ does not matter because the indices $j, k, \ldots$ are contracted with δ_{jk}. $(\Gamma_a)_{jk} = \Gamma_{ajk}$ takes values in so(D) that it can be represented by anti-symmetric matrices.

Our aim is to rewrite the constraint G_{jk} in the form of a so-called Gauß constraint of a SO(D) gauge theory. To be able to do this, we need to restrict to $D = 3$ because E_j^a transforms in the defining representation of so(D), but Γ_{ajk} transforms in the adjoint representation of so(D) and only in $D = 3$ dimensions both of them are identical.

Constant Weyl transformation : Now we consider the constant Weyl transformation which is only a rescaling of K_a^j and E_j^a according to the maps

$$\begin{aligned} K_a^j &\mapsto \beta K_a^j \\ E_j^a &\mapsto \frac{E_j^a}{\beta} =: {}^{(\beta)}E_j^a \ , \end{aligned} \tag{108}$$

where $\beta \neq 0$ is called ***Immirzi parameter***. The rotational constraint G_{jk} in $D = 3$ dimensions can equivalently be written as $G_j = \epsilon_{jk\ell} K_a^k E_\ell^a$ and is invariant under such a rescaling.

Affine transformation: From $D_a e_j^b = 0$ follows that $D_a E_j^b = 0$ which in detail has the form

$$D_a E_j^a = \partial_a E_j^a + \Gamma_{aj}^k E_k^a = \partial_a E_j^a + \epsilon_{jk\ell}\Gamma_a^k E_\ell^a = 0, \tag{109}$$

where we defined $\Gamma_a^\ell := \frac{1}{2}\epsilon_{j\ell k}\Gamma_a^{jk}$ which is an isomorphism between antisymmetric tensors of second rank and vectors in Euclidean space. Solving $D_a e_j^b = 0$ or respectively $D_a E_j^b = 0$ for Γ_a^k leads to, see [9, 80],

$$\Gamma_a^k = \frac{1}{2} e_j^b \epsilon^{kij} \left(\partial_a e_{bi} - \partial_b e_{ai} - e_{a\ell} e_i^c \partial_b e_c^\ell\right). \tag{110}$$

From eq. (110) we can conclude that Γ_j^k as a function of E_j^a is invariant under the rescaling, that is ${}^{(\beta)}\Gamma_a^j := \Gamma_a^j\left({}^{(\beta)}E\right) = \Gamma_a^j$. Therefore, the derivative D_a is independent of the rescaling, i.e. $D_a\ {}^{(\beta)}E_j^a = 0$ and by adding a zero we can write the rotational constraint as

$$G_j = \partial_a\left(\frac{E_j^a}{\beta}\right) + \epsilon_{jk\ell}\left[\Gamma_a^k + \beta K_a^k\right]\left(\frac{E_\ell^a}{\beta}\right) =: {}^{(\beta)}\mathcal{D}_a\ {}^{(\beta)}E_j^a \tag{111}$$

which motivates us to define the new covariant derivative ${}^{(\beta)}\mathcal{D}_a$. When we take a closer look at eq. (111), we recognize that this relation has the same structure as a Gauß constraint for a SU(2) gauge theory. From this moment on we will denote G_j as the ***Gauß constraint***.

We arrived at the point where we can introduce the ***Sen-Ashtekar-Immirzi-Barbero connection*** (historical order) or shortly just new connection

$${}^{(\beta)}A_a^j := \Gamma_a^j + \beta K_a^j. \tag{112}$$

The exact name depends on the choice of β: Sen connection for $\beta = \pm i$, $G_j = 0$, Ashtekar connection for $\beta = \pm i$, Immirzi connection for general complex β and Barbero connection for real β. However, due to Ashtekar's seminal work [86, 87, 91, 92], often it is only referred to as ***Ashtekar connection***.

In summary the SU(2) connection ${}^{(\beta)}A_a^j$ and the ***non-Abelian electric fields*** ${}^{(\beta)}E_j^a$, with spatial indices $a = 1, 2, 3$ and SU(2) indices $j = 1, 2, 3$ describe the phase space of an SU(2)-Yang-Mills gauge theory. The symplectic structure of the phase space is defined by the following Poisson brackets:

$$\begin{aligned}\{{}^{(\beta)}E_j^a\,(x), {}^{(\beta)}A_b^k\,(y)\} &= \frac{\kappa}{2}\delta_b^a\delta_j^k\delta^{(3)}(x,y) \\ \{{}^{(\beta)}E_j^a\,(x), {}^{(\beta)}E_k^b\,(y)\} &= \{{}^{(\beta)}A_a^j\,(x), {}^{(\beta)}A_b^k\,(y)\} = 0.\end{aligned} \tag{113}$$

In addition to the Hamiltonian and the spatial diffeomorphism constraint, the phase space complies with the Gauß constraint

$$G_j = {}^{(\beta)}\mathcal{D}_a\ {}^{(\beta)}E_j^a = \partial_a\ {}^{(\beta)}E_j^a + \epsilon_{jk\ell}\ {}^{(\beta)}A_a^k\ {}^{(\beta)}E_\ell^a = 0. \tag{114}$$

Now we want to consider the functions $\mathbb{Q}_{ab}$, $\mathbb{P}^{ab}$ in terms of ${}^{(\beta)}A_a^j$ and ${}^{(\beta)}E_j^a$, respectively E_j^a, defined by

$$\begin{aligned}\mathbb{Q}_{ab}(A,E) &:= |\det(E)|E_a^jE_b^k\delta_{jk}, \\ \mathbb{P}^{ab}(A,E) &:= \frac{2}{|\det(E)|}E_j^aE_k^d\delta^{jk}\left({}^{(\beta)}A_{[d}^\ell - \Gamma_{[d}^\ell\right)\delta_{c]}^bE_\ell^c\end{aligned} \tag{115}$$

with $k_{[a}s_{b]} := (k_as_b - s_bk_a)$. It is possible to show that they have the same Poisson brackets as the ADM variables q_{ab}, p^{ab} modulo $G_j = 0$.

Even more, when we use the identity $|\det(E)| = (\det(e))^2 = q$, we can directly identify $\mathbb{Q}_{ab}$ with q_{ab}

$$\mathbb{Q}_{ab} = |\det(E)|E_a^jE_b^k\delta_{jk} = q\frac{e_a^j}{\sqrt{q}}\frac{e_b^k}{\sqrt{q}}\delta_{jk} = q_{ab} \tag{116}$$

and analogous $\mathbb{Q}^{ab}$ with q^{ab}.

As shown in [9, 80] an explicit calculation of the Poisson brackets results in

$$
\begin{aligned}
&\{\mathbb{Q}_{ab}(x),\mathbb{Q}_{cd}(y)\} = 0, \\
&\{\mathbb{P}^{ab}(x),\mathbb{Q}_{cd}(y)\} = \kappa\delta^a_{(c}\delta^b_{d)}\delta^{(3)}(x,y)\,, \\
&\{\mathbb{P}^{ab}(x),\mathbb{P}^{cd}(y)\} = -\frac{\kappa}{4}\sqrt{q}\left(\mathbb{Q}^{bc}\tilde{G}^{ad}+\mathbb{Q}^{bd}\tilde{G}^{ac}+\mathbb{Q}^{ac}\tilde{G}^{bd}+\mathbb{Q}^{ad}\tilde{G}^{bc}\right)\delta^{(3)}(x,y)
\end{aligned}
\tag{117}
$$

with

$$
\tilde{G}^{ab} := \mathbb{Q}^{ac}\mathbb{Q}^{bd}G_{jk}e^j_c e^k_d = -qq^{ac}q^{bd}G_{cd}, \tag{118}
$$

for G_{ik} see eq. (103). Eq. (117) reproduces the Poisson brackets of q_{ab}, p^{ab} on the hypersurface where the Gauß constraint is satisfied, i.e. $G_{jk}=0$ or $G_j=0$ and we used that $\mathbb{Q}^{ab}\mathbb{Q}_{bc}=\delta^a_c$.

Next we need to express the diffeomorphism constraint C_a and the Hamiltonian constraint C in terms of the densitized triad E^a_j and the new connection ${}^{(\beta)}A^j_a$. Remember that C_a is given by

$$
C_a = -2q_{ac}D_b p^{bc} = 2sD_b\left[K^j_a E^b_j - \delta^b_a K^j_c E^c_j\right] \tag{119}
$$

for $s=-1$. The curvatures R^j_{ab} and F^j_{ab} connected with D_a and ${}^{(\beta)}\mathcal{D}_a$ can be defined via

$$
\begin{aligned}
[D_a, D_b]\,\upsilon_j &=: R_{abjk}\upsilon^k = \epsilon_{j\ell k}R^\ell_{ab}\upsilon^k, \\
\left[{}^{(\beta)}\mathcal{D}_a\,,\,{}^{(\beta)}\mathcal{D}_b\right]\upsilon_j &=: {}^{(\beta)}F_{abjk}\;\upsilon^k = \epsilon_{j\ell k}\;{}^{(\beta)}F^\ell_{ab}\;\upsilon^k
\end{aligned}
\tag{120}
$$

which explicitly expressed in terms of Γ^j_a and ${}^{(\beta)}A^j_a$ or K^j_a respectively read

$$
\begin{aligned}
R^j_{ab} &= 2\partial_{[a}\Gamma^j_{b]} + \epsilon_{jk\ell}\Gamma^k_a\Gamma^\ell_b, \\
{}^{(\beta)}F^j_{ab} &= 2\partial_{[a}\;{}^{(\beta)}A^j_{b]} + \epsilon_{jk\ell}\;{}^{(\beta)}A^k_a\;{}^{(\beta)}A^\ell_b \\
&= R^j_{ab} + 2\beta D_{[a}K^j_{b]} + \beta^2\epsilon_{jk\ell}K^k_a K^\ell_b.
\end{aligned}
\tag{121}
$$

Multiplication of ${}^{(\beta)}F^j_{ab}$ with ${}^{(\beta)}E^b_j$ leads to

$$
\begin{aligned}
{}^{(\beta)}F^j_{ab}\;{}^{(\beta)}E^b_j &= \frac{1}{\beta}R^j_{ab}E^b_j + 2\beta D_{[a}\left(K^j_{b]}E^b_j\right) + \beta K^j_a G_j \\
&= -sC_a + {}^{(\beta)}K^j_a\;G_j,
\end{aligned}
\tag{122}
$$

where we used that the first term $R^j_{ab}E^b_j=0$ vanishes as shown in [9] with the help of the ***algebraic Bianchi identity***.

The Hamiltonian constraint $C(x)$ is given by

$$
\begin{aligned}
C &= -\frac{s\kappa}{\sqrt{q}}\left[q_{ac}q_{bd}-\frac{1}{2}q_{ab}q_{cd}\right]p^{ab}p^{cd} - \sqrt{q}R^{(3)} \\
&= -s\sqrt{q}\left(K_{ab}K^{ab}-K^2\right) - \sqrt{q}R^{(3)} \\
&= -\frac{s}{\sqrt{q}}\left(K^k_a K^j_b - K^j_a K^k_b\right)E^a_j E^b_k - \sqrt{q}R,
\end{aligned}
\tag{123}
$$

where we defined $q := \det(q_{ab})$ and $R := R^{(3)}$. Now let us multiply ${}^{(\beta)}F^j_{ab}$ with $\epsilon^{jk}_{\ell}\ {}^{(\beta)}E^a_k\ {}^{(\beta)}E^b_\ell$ this gives

$$\begin{aligned}
{}^{(\beta)}F^j_{ab}\ \epsilon^{k\ell}_j\ {}^{(\beta)}E^a_k\ {}^{(\beta)}E^b_\ell &= -q\frac{R^{k\ell}_{ab}e^a_k e^b_\ell}{\beta^2} - 2\frac{E^a_j D_a G_k \delta^{kj}}{\beta} + \left(K^j_a E^a_j\right)^2 - \left(K^j_b E^a_j\right)\left(K^k_a E^b_k\right) \qquad (124)\\
&= -q\frac{R}{\beta^2} + \left(K^j_a E^a_j\right)^2 - \left(K^j_b E^a_j\right)\left(K^k_a E^b_k\right) - 2\frac{E^a_j D_a G_k \delta^{kj}}{\beta}\\
&= \frac{\sqrt{q}}{\beta^2}\left[-\sqrt{q}R - \beta^2\frac{\left(K^j_b E^a_j\right)\left(K^k_a E^b_k\right) - \left(K^j_a E^a_j\right)^2}{\sqrt{q}}\right] - 2\frac{E^a_j D_a G_k \delta^{kj}}{\beta}\\
&= \frac{\sqrt{q}}{\beta^2}\left[-\sqrt{q}R + \beta^2\left(sC + s\sqrt{q}R\right)\right] - 2\ {}^{(\beta)}E^a_j\ D_a G_k \delta^{kj}\\
&= s\sqrt{q}\left[C + \left(1 - \frac{s}{\beta^2}\right)\sqrt{q}R\right] - 2\ {}^{(\beta)}E^a_j\ D_a G_k \delta^{kj}.
\end{aligned}$$

Here we used that $s = \pm 1$, that is for Lorentzian signature we have $s = -1$ and for Euclidean signature we have $s = +1$, consequently $s^2 = 1$. In summary in terms of ${}^{(\beta)}E^a_j$, R and ${}^{(\beta)}F^j_{ab}$ we obtain for the constraints modulo gauge transformations $G_j = 0$ the expressions

$$\begin{aligned}
C_a &= -s\left({}^{(\beta)}F^j_{ab}\ {}^{(\beta)}E^b_j\right) \qquad (125)\\
C &= \frac{s}{\sqrt{q}}\left({}^{(\beta)}F^j_{ab}\ \epsilon^{jk}_\ell\ {}^{(\beta)}E^a_k\ {}^{(\beta)}E^b_\ell\right) - \left(1 - \frac{s}{\beta^2}\right)\sqrt{q}R
\end{aligned}$$

To get rid of the additional $\frac{s}{\beta^2}\sqrt{q}R$ term we see that we can make the following choices to simplify the form of C:

1. For Euclidean signature $s = 1$: choose $\beta = \pm 1$, but this does not match with our physical assumptions.

2. For Lorentzian signature $s = -1$: choose $\beta = \pm i$, however then ${}^{(\beta)}A^j_a$ is no longer an SU(2) connection but rather $\mathrm{SL}(2,\mathbb{C})$ valued. The problem is that $\mathrm{SL}(2,\mathbb{C})$ is a non-compact gauge group for which we cannot apply the quantization techniques used in LQG, since they heavily rely on the compactness of the gauge group. Furthermore, it is also complicated to implement reality conditions.

We will come back to this obstacle when we actually need to quantize the Hamiltonian constraint. For later use we define here the ***Euclidean Hamiltonian*** density for $s = 1$ and $\beta = 1$ as

$$C_{\mathrm{E}} := \frac{1}{\sqrt{|\det(E)|}}\left({}^{(1)}F^j_{ab}\ \epsilon^{jk}_\ell E^a_k E^b_\ell\right) = -\sqrt{q}\left(K_{ab}K^{ab} - K^2\right) - \sqrt{q}R \qquad (126)$$

with $q = |\det(E)|$.

Remark: In the literature it is more common to define $A^j_a := {}^{(\beta)}A^j_a := \Gamma^j_a + \beta K^j_a$ and instead of ${}^{(\beta)}E^a_k$ to use E^a_j, then the Poisson bracket has the form

$$\{E^a_j(x), A^k_b(y)\} = \frac{\kappa\beta}{2}\delta^a_b\delta^k_j\delta^{(3)}(x,y). \qquad (127)$$

We will stick to this convention in the following.

2 Quantum Theory

For a given, possibly infinite-dimensional constrained symplectic manifold $(\mathcal{M}, \omega)$ with strong symplectic structure ω modeled on a Banach space (complete, normed vector space) and first class constraints C_I, I being an element of a finite index set, the canonical quantization program can be split into three main steps that we are going to describe in the following sections. In our presentation we closely follow the one given in [9]. For mathematical details on differential geometry, we refer to [93, 94]. The three steps we need to perform in order to arrive at our quantum theory consist of:

1. Choice of the classical Poisson*-subalgebra $\mathfrak{P}$.
2. Choice of the quantum *-algebra $\mathfrak{Q}$.
3. Finding a representation of the quantum *-algebra $\mathfrak{Q}$.

2.1 Choice of the Classical Poisson*-subalgebra $\mathfrak{P}$

We are looking for a set of global coordinates that coordinatize the phase space in such a way that all functions on $\mathcal{M}$ can be expressed in terms of these ***"elementary functions"***. Furthermore, these elementary functions need to form a closed Poisson *-subalgebra of the full Poisson *-algebra $C^\infty(\mathcal{M})$ of smooth functions on $\mathcal{M}$ to be able to represent the Poisson bracket times $i\hbar$ as a commutator in the quantum theory. Here * stands for an involution map. In general an ***involution*** on an algebra $\mathfrak{A}$ is an antilinear automorphism on $\mathfrak{A}$ with the properties: $(z_1 a + z_2 b)^* := \bar{z}_1 a^* + \bar{z}_2 b^*$, $(ab)^* = b^* a^*$, $(a^*)^* = a$ with $a, b \in \mathfrak{A}$ and $z_1, z_2 \in \mathbb{C}$. For $\mathfrak{A} = \mathbb{C}$ and $z \in \mathbb{C}$ the involution is just the complex conjugation, that is $\bar{z} = z^*$.
The closed Poisson *-subalgebra can be found by considering any set of elementary functions which ***separate*** the points of $\mathcal{M}$, i.e. for $x, y \in \mathcal{M}$ with $x \neq y$ the elementary function f satisfies $f(x) \neq f(y)$, and then construct from the elementary functions and their complex conjugates the smallest possible Poisson algebra they can generate. The result will be a separating ***Poisson*-subalgebra $\mathfrak{P}$ on $\mathcal{M}$***.

The choice of the separating elementary functions can be guided by the requirement that they should have a simple transformation behaviour under gauge transformations (symmetries) of the system in consideration and a symplectic structure that is as simple as possible, which in the ideal case reduces to the canonical Poisson bracket. In case that $\mathcal{M}$ has the structure of a cotangent bundle over a configuration space $\mathcal{C}$, that is $\mathcal{M} = T^*\mathcal{C}$, which complies with General Relativity, we can determine $\mathfrak{P}$ by the subsequent procedure.

Select an algebra of smooth functions (possibly smeared in case of a field theory) $\mathrm{Fun}(\mathcal{C})$ on the configuration space $\mathcal{C}$. Next determine the Hamiltonian vector fields of the (smeared) momentum functions on $\mathcal{M}$ which should be sufficiently smooth defined to act as vector fields $V(\mathcal{C})$ on $\mathcal{C}$ that preserve $\mathrm{Fun}(\mathcal{C})$. Having found $\mathrm{Fun}(\mathcal{C})$ and $V(\mathcal{C})$, we can define a Lie algebra structure on the product space $\mathrm{Fun}(\mathcal{C}) \times V(\mathcal{C})$ by

$$\{(f, \nu), (f', \nu')\} := (\nu[f'] - \nu'[f], [\nu, \nu']) \tag{128}$$

for $f \in \mathrm{Fun}(\mathcal{C})$ and $\nu[f] \in V(\mathcal{C})$ is the vector field acting on f. Since this expression is a classical one, it is sometimes called a Poisson bracket despite the fact that it actually defines a Lie bracket. The Poisson *-subalgebra $\mathfrak{P}$ is then the closed ***Lie subalgebra*** of $\mathrm{Fun}(\mathcal{C}) \times V(\mathcal{C})$ generated by the elements (f, ν) and their complex conjugate algebra elements (f^*, ν^*).

2.1.1 Holonomy-Flux-Algebra

In LQG the holonomies, respectively the smooth cylindrical functions and the Hamiltonian vector fields of the fluxes are the elementary phase space functions that separate the points of $\mathcal{M}$ and build a Poisson*-subalgebra, the so-called ***holonomy-flux algebra***. In the following we want to introduce these quantities in detail. We follow [9, 11, 80].

Our description of the classical theory ended with the definition of the Ashtekar variables, i.e. the densitized triads (electric fields) $E^a_j(x)$ and the new connections $A^b_k(y)$ which satisfy the Poisson algebra

$$\{E^a_j(x), A^k_b(y)\} = \frac{\kappa\beta}{2}\delta^a_b\delta^k_j\delta^{(3)}(x,y). \tag{129}$$

Naively, we would like to go over to the quantum theory by making the replacement $\{.,.\} \to \frac{1}{i\hbar}[.,.]$. If this were possible, we would have the commutator

$$\left[E^a_j(x), A^k_b(y)\right] = i\hbar\frac{\kappa\beta}{2}\delta^a_b\delta^k_j\delta^{(3)}(x,y)\mathbb{1}, \tag{130}$$

here we used the same symbols for classical variables and their corresponding quantum operators and $\mathbb{1}$ denotes the identity operator. Notice that $\hbar\kappa = \ell_p^2$ is the Planck area of order 10^{-68}cm^2. Unfortunately, in LQG this naive quantization does not work, since $E^a_j(x)$ and $A^k_b(y)$ become operator valued distributions and not operators. Even more, later we will reexpress classical variables, for example the Hamiltonian constraint, in terms of products of Poisson brackets of $E^a_j(x)$ and $A^k_b(y)$ or objects derived from them. All of this means that if we try to quantize $E^a_j(x)$ and $A^k_b(y)$ directly, distributions and products thereof will enter which are singular quantities.

To avoid this problem, we need to find suitable smearings of $E^a_j(x)$ and $A^k_b(y)$ to be able to define the corresponding quantum operators. Three dimensional smearings lead to background depedencies or non closing algebras, that is why one uses lower dimensional smearings, see [9].

Since $E^a_j(x)$ is dual to the pseudo-two form $\epsilon_{abc}E^c_j(x)$, we try to smear the pseudo-two form in two dimensions along an oriented surface S which gives rise to the ***non-Abelian flux***

$$E_n(S) := \int_S n^j\,(*E)_j = \int_S \mathrm{d}x^a \wedge \mathrm{d}x^b \epsilon_{abc}E^c_j n^j, \tag{131}$$

where n^j is a Lie algebra valued smearing field. In the equation above occurs the so-called ***Hodge dual*** $(*E)_j := \epsilon_{aa_1\ldots a_{D-1}}E^a_j \mathrm{d}x^{a_1} \wedge \mathrm{d}x^{a_{D-1}}$ of E_j.

Analogous we try to smear $A^k_b(x)$ in one dimension along a path (edge) $e(t)$ parametrized by $t \in [0,1]$ which leads to

$$A(e) := \int_e \mathrm{d}x^a A_a(x) = \int_0^1 \mathrm{d}t\,\dot{e}^a(t)A^j_a(e(t))\tau_j \tag{132}$$

However, $A(e)$ is not invariant under SU(2) gauge transformations and also other classical variables written in terms of $A(e)$ cannot be written in a manifestly SU(2) invariant way. For this reason we will instead introduce the so-called ***holonomies*** $h_e(A)$.

Before we come to the definition of the holonomy we mention that in the upcoming we will only consider piecewise analytic paths and piecewise analytic surfaces. A ***piecewise analytic path*** p consists of finitely many real analytic segments, called ***edges*** e, i.e. $e(t) = \sum_{s=0}^{\infty}\frac{(t-s)^n}{n!}e^{(n)}(s)$, $\exists\ \forall s \in [0,1]$, which meet in their boundaries, called vertices v which are the beginning $b(e)$ or the endpoint $f(e)$ of an edge e. We define a ***graph*** γ to be a finite collection of edges and denote by $E(\gamma)$ the ***set of edges*** of γ and by $V(\gamma) = \{b(e), f(e); e \in E(\gamma)\}$ the ***set of vertices*** of γ. A ***piecewise analytic surface*** S is a finite union of entire analytic surfaces, called faces F, satisfying the following conditions, for a generalization see [95]:

1. A face is an entire analytic, connected, embedded $(D-1)$-dimensional manifold in σ (without a boundary).
2. The faces F are mutually disjoint. Their closures $\bar{F}$ intersect at most at their boundaries which are piecewise analytic $(D-2)$-dimensional submanifolds. For $D = 3$ the boundaries themselves are piecewise analytic paths.
3. The union of the faces is a connected $(D-1)$-dimensional submanifold (without a boundary) of differetiability class C^0, i.e. continous.
4. The closure of the surface $\bar{S}$ is contained in a compact, $(D-1)$-dimensional C^0 submanifold with boundary.
5. S is ***orientable***, i.e. it exists an open neighbourhood U of S, such that $U - S = U_+ \cup U_-$ is a union of disjoint, connected, open non-empty sets U_+ and U_-. In this sense we are able to distinguish between "above the surface" U_+ and "beyond the surface" U_-.

Later one usually sticks to ***semianalytic*** structures instead of piecewise analytic structures, which is important for the uniqueness proof of the representation of the holonomy-flux algebra, for details on semianalytic structures and the uniqueness proof see [95]. We will not give a precise definition of semianalytic here but we want to explain the arguments for using semianalytic instead of piecewise analytic structures. The main point is the locality or conservation of structure on lower-dimensional subsets. Piecewise analytic paths or surfaces will stay piecewise analytic on subsets of the same dimension, but piecewise analycity might be violated on subsets of lower dimension. Semianalytic carries over even to subsets of lower-dimensionality. At points of non-analycity a piecewise analytic path has to be continuous while a semianalytic path has to be C^n for $n > 0$, $n \in \mathbb{N}$.

Now we can go on constructing our elementary functions of our classical Poisson*-subalgebra $\mathfrak{P}$.

Definition [9, 80]: Holonomy 2.1.1. *Let $A \in \mathcal{A}$ be a smooth* SU(2) *connection, where $\mathcal{A}$ denotes the set of all smooth connections and let $e : [0,1] \to \sigma$, $t \mapsto e(t)$ be a one dimensional path in σ (here we denote the path with e and not only a single edge). Then the **holonomy** of A along e is defined as the unique solution $h_e(A) := h_e(0,t)|_{t=1} = h_e(0,1)$ of the so-called **parallel transport equation** which denotes the ordinary differential equation*

$$\frac{\mathrm{d}}{\mathrm{d}t} h_e(0,t) = h_e(0,t) A(e(t)) \tag{133}$$

with

$$A(e(t)) := \dot{e}^a(t) A_a(e(t)) := \dot{e}^a(t) A_a^j(e(t)) \tau_j \tag{134}$$

for $\tau_j = -i\sigma_j$, σ_j with $j = 1,2,3$ being the Pauli matrices and

$$h_e(0,0) = h_e(0,t)|_{t=0} = \mathbb{1}_{\mathrm{SU}(2)}. \tag{135}$$

i)The explicit general solution to the parallel transport equation is a path ordered exponential

$$h_e(0,t) = \mathcal{P}\exp\left(\int_0^t \mathrm{d}s\, A(e(s))\right) = \mathcal{P}\exp\left(\int_0^t \mathrm{d}s\, \dot{e}^a(s)A_a(e(s))\right) \tag{136}$$
$$= \mathbb{1}_{\mathrm{SU}(2)} + \sum_{n=1}^{\infty}\int_0^t \mathrm{d}s_n \int_0^{s_n}\mathrm{d}s_{n-1}\ldots\int_0^{s_2}\mathrm{d}s_1\, A(e(s_1))\ldots A(e(s_n)),$$

where in the Taylor expansion the latest parameter value is ordered to the right, i.e. $0 < s_1 < \ldots < s_n < t$ *. This can equivalently be written as*

$$h_e(0,t) = \mathbb{1}_{\mathrm{SU}(2)} + \sum_{n=1}^{\infty}\frac{1}{n!}\int_0^t \mathrm{d}s_n \int_0^t \mathrm{d}s_{n-1}\ldots\int_0^t \mathrm{d}s_1\, \mathcal{P}\left(A(e(s_1))\ldots A(e(s_n))\right). \tag{137}$$

ii) Let g be an element of the Lie group SU(2). Under SU(2) gauge transformation the connection transforms as $A^g = -\mathrm{d}gg^{-1} + gAg^{-1}$. From this we can derive the transformation behaviour of the holonomy to be $h_e(A) \mapsto h_e^g(A) = g(b(e))h_e(A)g(f(e))^{-1}$, where $b(e) := e(0)$ is the beginning and $f(e) := e(1)$ is the final point of the path.

iii) Impose that $e_1 \cap e_2 = f(e_1) = b(e_2)$, then one can parametrize the composed, connected path by $(e_1 \circ e_2)(t) := \begin{cases} e_1(2t), & 0 \le t \le \frac{1}{2} \\ e_2(2t-1), & \frac{1}{2} \le t \le 1 \end{cases}$ and $h_{(e_1\circ e_2)} = h_{e_1}h_{e_2}$.

iv) The inverse path (orientation changed) is obtained from $e^{-1}(t) = e(1-t)$ and the corresponding holonomy is $h_{e^{-1}} = h_e^{-1}$

v) $h_e^{*T} = h_e^{-1}$ and $\det(h_e) = 1$ for $h_e \in \mathrm{SU}(2)$.

The definition of holonomies can also be generalized to complex valued functions of the holonomies, the so-called ***cylindrical functions***.

Definition [9, 80]: Cylindrical Function 2.1.2. *Let G be a compact group, usually $G = \mathrm{SU}(2)$ in LQG. Consider a graph γ, where the number of edges is given by $|E(\gamma)|$ and define a projective map $p_\gamma : \mathcal{A} \to G^{|E(\gamma)|}$; $A \mapsto \{h_e[A]\}_{e\in E(\gamma)}$ A function f is said to be **cylindrical over a graph** γ iff there exists a function $f_\gamma : G^{|E(\gamma)|} \to \mathbb{C}$ such that f is gained from the composition $f = f_\gamma \circ p_\gamma = p_\gamma^* f_\gamma$, where p_γ^* denotes the pull-back of p_γ. The functions cylindrical over γ are denoted by Cyl_γ and the *-algebra of cylindrical functions is defined by $Cyl := \bigcup_{\gamma\in\Gamma} Cyl_\gamma$, where the involution is the complex conjugation. The subalgebras Cyl^n, $n = 0, 1, 2\ldots, \infty$ of Cyl consist of functions of the form $f = f_\gamma \circ p_\gamma$ with $f_\gamma \in C^{(n)}(G^{|E(\gamma)|})$, where we denote the subalgebra of smooth cylindrical functions by Cyl^∞.*

To be more precise a cylindrical function is actually not one function but an equivalence class of complex valued functions. Imagine you have one graph which consists of only one edge $\gamma = \{e\}$ and a function cylindrical with respect to γ and another graph $\gamma' = e_1, \ldots, e_n$ whose edges satisfy $e = e_1 \circ \ldots \circ e_n$ for $n \in \mathbb{N}$. In this case the holonomy can be expressed as $h_e = h_{(e_1\circ\ldots e_n)} = h_{e_1}\cdot\ldots\cdot h_{e_n}$, see 2.1.1 and therefore the function is also cylindrical with respect to γ'.

In the calculation of the Poisson bracket of holonomies and fluxes we need to split a path p into edges depending on their orientation with respect to the surface. It is possible to classify each edge as a member of one of the four following categories:

- out: The edge e_{out} has no intersection points with the surface S.
- in : The edge e_{in} is entirely contained in the surface S.
- up: The edge e_{up} is contained in U_+ (above the surface), its intersection point with S is equal to its beginning with outgoing orientation from the intersection point.
- down: The edge e_{down} is contained in U_- (beyond the surface), its intersection point with S is equal to its beginning with outgoing orientation from the intersection point.

To actually calculate the Poisson bracket between holonomies and fluxes one has to smear the classical quantities in D (here $D = 3$) directions by smooth functions and then perform a limiting process to reduce the actual smearing dimension to get back holonomies and fluxes. Visually, this is done by putting a path inside a tube in case of holonomies and making a surface a section through a higher-dimensional surface in case of fluxes. Mathematically, this is accomplished by introducing tailored delta distributions in the smearing functions and integration then reassembles the holonomies and fluxes, for details on this see [9]. For piecewise analytic edges and piecewise analytic surfaces the Poisson bracket of holonomies and fluxes as defined in eq. (131) becomes, see [9, 12],

$$\{E_n(S), h_e\} = \begin{cases} \frac{\beta\kappa}{2} h^{-1}_{e_{\text{down}}} n^j(p)\tau_j h_{e_{\text{up}}} \text{ for a single transversal intersection } S \cap e = \{p\} \\ \qquad 0 \text{ if } S \cap e = \varnothing \end{cases}, \tag{138}$$

where $\tau_j = -i\sigma_j$, σ_j with $j = 1, 2, 3$ being the Pauli matrices. The edge e in this case is composed of e_{up} and e_{down} as $e = e^{-1}_{\text{down}} \circ e_{\text{up}}$, where the intersection point with the surface S is the beginning point of e_{up} and e^{-1}_{down}. If one changes the orientation of the surface S, e_{up} and e_{down} will change their roles. This makes it possible to simplify the Poisson bracket of holonomies and fluxes by making use of edges of type up only, leading to

$$\{E_n(S), h_e\} = \frac{\beta\kappa}{4}\sigma(S, e)\left[n^j(b(e))\tau_j h_e\right] \tag{139}$$

with $b(e)$ being the beginning of the edge e and

$$\sigma(S, e) := \begin{cases} +1, & e_{\text{up}} \\ -1, & e_{\text{down}} \\ 0, & e_{\text{in}},\ e_{\text{out}} \end{cases}.$$

Notice that we have $\frac{\beta\kappa}{4}$ here and not $\frac{\beta\kappa}{2}$. We gain a factor 1/2 by splitting an edge e going through the surface in "up" and "down" pieces and consider them to be of only one type, namely type up, because instead of an integral $\int_{-\infty}^{\infty} \mathrm{d}t\, \delta(t) = 1$ we have an integral $\int_0^{\infty} \mathrm{d}t\, \delta(t) = 1/2$.

Since in the general quantization process we consider fluxes and cylindrical functions, we lift the Poisson bracket to the case where we generalize the action of $E_n(S)$ to smooth cylindrical functions

$$\{E_n(S), f\} = \frac{\beta\kappa}{4}\sum_{e\in E(\gamma)} \sigma(S, e)\left[n^j(b(e))\tau_j h_e\right]_{mn} \frac{\partial f_\gamma}{\partial(g_e)_{mn}}\Big|_{g_e=h_e}, \tag{140}$$

where m, n are matrix indices. It is possible to further rewrite the Poisson bracket of the flux and a cylindrical function by making use of the definition of left and right invariant vector fields on SU(2). As a preparation we introduce the ***left*** λ_g ***and right*** ρ_g ***translations*** [96] by

$$\begin{aligned} \lambda_g &: G \to G, \quad h \mapsto gh, \\ \rho_g &: G \to G, \quad h \mapsto hg, \end{aligned} \tag{141}$$

where $g, h \in G$ and G is a topological group. In case that G is a Lie group λ_g and ρ_g are diffeomorphisms.

Definition [96]: Left and Right Invariant Vector Fields 2.1.3. *Let G be a matrix Lie group with Lie algebra $\mathfrak{L}(G)$ and left λ_g and right ρ_g translation diffeomorphisms.*

For $B \in \mathfrak{L}(G)$, $g := \exp(tB)$ and $f \in Cyl^\infty$ we define

$$(R_B f)(h) := \frac{d}{dt}|_{t=0} f(gh) = \frac{d}{dt}|_{t=0} \left(\lambda_g^* f\right)(h) \tag{142}$$

*to be the generator of left translations in B direction, called the **right invariant vector field**.*

$$(L_B f)(h) := \frac{d}{dt}|_{t=0} f(hg) = \frac{d}{dt}|_{t=0} \left(\rho_g^* f\right)(h) \tag{143}$$

*to be the generator of right translations in B direction, called the **left invariant vector field**. Here $*$ stands for the pull-back of a diffeomorphism.*

The names right and left invariant vector fields come from the fact that $\lambda_h \rho_g = \rho_g \lambda_h$, therefore the generator of left translations $\rho_h^* R_B = R_B \rho_h^*$ is right translation invariant and the generator of right translations $\lambda_h^* L_B = L_B \lambda_h^*$ is left translation invariant.

Using the definition of the right invariant vector field with $B = \tau_j$ and $R_j := R_{\tau_j}$ the Poisson bracket of the flux and a smooth cylindrical function becomes

$$\{E_n(S), f\} = \frac{\beta\kappa}{4} \sum_{e \in E(\gamma)} \sigma(S, e) n^j(b(e)) R_j^e f_\gamma =: Y_n(S) \cdot f. \tag{144}$$

By inspection of the right hand side of the equation, we see that the Poisson bracket with the flux defines a derivation on the space of smooth cylindrical functions denoted by $Y_n(S) \cdot f$ and that R_j^e acts only on the e-th copy of SU(2) in f_γ. From now on we will consider the ***Hamiltonian vector fields*** $Y_n(S) = \{E_n(S), .\}$ instead of the $E_n(S)$. Notice that the Poisson bracket $\{E_n(S), E_n'(S')\}$ does not vanish. This comes from the smearing of E_j^a in two instead of three dimensions, but a smearing in three dimension would lead to a non closing subalgebra and to a dependence on the background metric. As a consequence, the commutator $[Y_n(S)[f], Y_{n'}(S')[f]]$ is also not supposed to vanish.

Consider the Lie *-algebra $\mathfrak{K}$ with elements $\ell := (f, Y_n(S))$ in $\mathrm{Cyl}^\infty \times V(\mathrm{Cyl}^\infty)$ with smooth cylindrical functions $f \in \mathrm{Cyl}^\infty$ and smooth vector fields $Y_n(S)(f) \in \mathrm{Cyl}^\infty$ on them. The complex conjugate elements are given by $\ell^* = (f^*, Y_n(S)^*)$ and we can define a Lie bracket by

$$[\ell, \ell'] := (Y_n(S)(f') - Y_n(S)'(f), [Y_n(S), Y_n(S)']) \,. \tag{145}$$

Further, we define the closed Lie *-subalgebra $\mathfrak{L}$ of $\mathfrak{K}$ by taking into account only those elements of $\mathfrak{K}$ which are generated from the $(f, Y_n(S))$ elements by commutators. The resulting classical Poisson (Lie) *-subalgebra $\mathfrak{P} = \mathfrak{L}$ is known as the ***holonomy-flux algebra***.

2.2 Quantization of Holonomies and Fluxes

There is also some important subtlety about the class of spatial diffeomorphisms we need to mention before we go into the quantization. We restricted our paths and surfaces to be piecewise analytic (semianalytic). Now we want the diffeomorphisms to preserve these piecewise analytic (semianalytic) structures, since otherwise the spatial diffeomorphism would not implement an automorphism on the holonomy-flux algebra. If we consider the class of analytic diffeomorphism, the conservation of the piecewise analytic (semianalytic) structures could not be achieved. Entire analytic diffeomorphism are too global, since an entire analytic function is already completely determined by its values in an arbitrary small neighbourhood of any point $x \in \sigma$. This is why we move to the class of ***piecewise analytic (semianalytic) diffeomorphisms***. Piecewise analytic (semianalytic) diffeomorphisms are analytic everywhere except on lower-dimensional submanifolds of σ, where they are only differetiable for finitely many times, see [97, 98].

2.2.1 Choice of the Quantum *-algebra $\mathfrak{Q}$

Now we construct the abstract quantum *-algebra $\mathfrak{Q}(\mathfrak{P})$ based on the classical Poisson *-subalgebra $\mathfrak{P}$ following Dirac [16]. The construction will implement the classical Poisson (actually Lie) bracket structure on $\mathfrak{P}$ times $i\hbar$ as a commutation relations on $\mathfrak{Q}$ and the complex conjugation on $\mathfrak{P}$ more general as involution on $\mathfrak{Q}$.

We construct $\mathfrak{Q}$ from $\mathfrak{P}$ as follows: define the free tensor algebra $\mathfrak{F}(\mathfrak{P})$ over $\mathfrak{P}$ by

$$\mathfrak{F}(\mathfrak{P}) := \mathbb{C} \oplus \oplus_{n=1}^{\infty} \otimes_{k=1}^{n} \mathfrak{P} \tag{146}$$

with elements sometimes called ***blocks*** $a := (a_0, a_1, \ldots, a_n, \ldots)$. Here $a_0 \in \mathbb{C}$ and a_n is a linear combination of monomials sometimes called ***words*** $a_n = a_{1n} \otimes \ldots \otimes a_{nn}$ of elements $a_{kn} \in \mathfrak{P}$ of which all but finitely many vanish. The elements of the algebra are subject to the operations

a.) multiplication: $(a \otimes b)_n = \sum\limits_{k+l=n} a_k \otimes b_l$; $a_k \otimes b_l = a_{1k} \otimes \ldots \otimes a_{kk} \otimes b_{1l} \otimes \ldots \otimes b_{ll}$,

b.) addition: $(a + b)_n = a_n + b_n$,

c.) scalar multiplication: $(za)_n = za_n$; $za_n = za_{1n} \otimes \ldots \otimes a_{nn} = a_{1n} \otimes \ldots \otimes za_{nn}$, $z \in \mathbb{C}$,

d.) involution: $a^* = \bar{a}_0 \oplus \oplus_{n=1}^{\infty} a_n^*$; $a_n^* = \bar{a}_{nn} \otimes \ldots \otimes \bar{a}_{1n}$.

Finally, we define the two-sided ideal $\mathfrak{I}(\mathfrak{P})$ which consists of elements of the form

$$a_1 \otimes b_1 - b_1 \otimes a_1 - i\hbar\{a_1, b_1\} \tag{147}$$

with a_1, $b_1 \in \mathfrak{P}$. Then the quantum *-algebra $\mathfrak{Q}$ which is an enveloping algebra of the Poisson (Lie) *-subalgebra $\mathfrak{P}$ is given by the quotient algebra

$$\mathfrak{Q}(\mathfrak{P}) = \mathfrak{F}(\mathfrak{P}) / \mathfrak{I}(\mathfrak{P}). \tag{148}$$

For LQG let $\mathfrak{F}(\mathfrak{L})$ be the free *-algebra generated by $\mathfrak{L}$ whose elements (blocks) consist of finite linear combinations of words $w = (\ell_1 \ldots \ell_N)$ build from a finite sequence of elements ℓ_k of $\mathfrak{L}$, remember $\ell := (f, Y_n(S))$ and eq. (145). The underlying operations for multiplication and involution for the words take the form

- multiplication: $w \cdot w' = (\ell_1 \ldots \ell_N \ell'_1 \ldots \ell'_N)$.
- involution (complex conjugation): $w^* = (\bar{\ell}_N \ldots \bar{\ell}_1)$.

We introduce the two sided ideal $\mathfrak{I}(\mathfrak{L})$ in $\mathfrak{F}(\mathfrak{L})$ generated by elements of the form

$$\ell \cdot \ell' - \ell' \cdot \ell - i\hbar\,[\ell, \ell']\,, \tag{149}$$

where $\cdot$ is the multiplication in $\mathfrak{F}(\mathfrak{L})$ and $[\ell, \ell']$ is the commutator in $\mathfrak{L}$. Therefore, the quotient algebra of $\mathfrak{F}(\mathfrak{L})$ and $\mathfrak{I}(\mathfrak{L})$ defines the quantum*-algebra $\mathfrak{Q}(\mathfrak{L})$, i.e.

$$\mathfrak{Q}(\mathfrak{L}) = \mathfrak{F}(\mathfrak{L})/\mathfrak{I}(\mathfrak{L}). \tag{150}$$

This is an abstract way of saying that we implement the canonical commutation relations in $\mathfrak{Q}(\mathfrak{L})$.

2.2.2 Representation of the Quantum *-algebra $\mathfrak{Q}$

So far we have defined the quantum *-algebra on an abstract level, that is we are not dealing with operators acting on a Hilbert space $\mathcal{H}$ yet. To obtain operators that can act on a Hilbert space $\mathcal{H}$, we need to find a representation of the quantum Lie *-algebra $\mathfrak{Q}$. A ***representation*** in this case is a ****-morphism*** (linear map which preserves the * operation) between $\mathfrak{Q}$ and a subalgebra of the set of bounded operators on the Hilbert space $\mathcal{B}(\mathcal{H})$. In order to find a representation of $\mathfrak{Q}$, one usually does not consider the elements of $\mathfrak{P}$ directly, but bounded functions thereof which still separate the points of $\mathcal{M}$. These bounded functions are called ***Weyl elements*** and they give rise to bounded operators. The reason for considering the Weyl elements instead of considering elements $a \in \mathfrak{P}$ directly is that the $a \in \mathfrak{P}$ are classically unbounded and so the operators defined from them should be unbounded, i.e. they can only be defined on a dense domain. The problem is then that we might not be able to define different self-adjoint operators on a common and invariant dense domain in which case we might not be able to define the two-sided ideal $\mathfrak{I}(\mathfrak{P})$ by elements that satisfy eq. (147). For this reason, and since we know how to compose them, we consider the bounded Weyl functions instead.

Definition [9]: Weyl Functions 2.2.1. *Let $a \in \mathfrak{P}$ be a real-valued unbounded element of $\mathfrak{P}$ and let $1_{\mathfrak{Q}}$ be the unit element in $\mathfrak{Q}$. The one-parameter family of unitary functions (operators), denoted as **Weyl functions**, see [9], are defined as*

$$W_t(a) := \exp(ita) \tag{151}$$

for $t \in \mathbb{R}$ and $a \in \mathfrak{P}$ which for $t \to 0$ approximates $1_{\mathfrak{Q}} + ita$. In eq. (147) we replace the elements a, $b \in \mathfrak{P}$ by their associated Weyl functions and their commutation relation becomes

$$W_s(a)W_t(b)W_{-s}(a) := W_t\left(\sum_{n=0}^{\infty} \frac{(is\hbar)^n}{n!}\{a, b\}_{(n)}\right) \tag{152}$$

with $(W_s(a))^* := W_{-s}(a) = (W_s(a))^{-1}$ and the iterated Poisson bracket $\{a, b\}_{(n+1)} = \{a, \{a, b\}_{(n)}\}$ and $\{a, b\}_{(0)} = b$.

In LQG the flux vector fields $Y_n(S)$ are unbounded functions while the cylindrical functions are already bounded, for details see [99], so for $t \in \mathbb{R}$ and $a = Y_n(S)$ the Weyl elements become

$$W_t^n(S) := e^{tY_n(S)} = e^{-it[iY_n(S)]} \tag{153}$$

with $n^j(x)n^k(x)\delta_{jk} = 1$. The commutation relation among $W_t^n(S) = \exp(t(Y_n(S)))$ and a smooth cylindrical function $f \in \mathrm{Cyl}^\infty$ reads

$$W_t^n(S) f\,(W_t^n(S))^{-1} = \sum_{m=0}^{\infty} \frac{t^m}{m!}\,[Y_n(S), f]_{(m)} = \sum_{m=0}^{\infty} \frac{t^m}{m!}\,(Y_n(S))^m f = W_t^n(S) \cdot f, \tag{154}$$

where we used the iterated commutator bracket $[Y_n(S), f]_{(0)} = f$ and $[Y_n(S), f]_{(m+1)} = \Big[Y_n(S), [Y_n(S), f]_{(m)}\Big]$. Inserting the expression for $Y_n(S)$ and $f = p_\gamma^* f_\gamma$

$$[W_t^n(S) \cdot f]\,(h) = [p_\gamma^* \prod_{e \in E(\gamma)} e^{t\sigma(S,e)n^j(b(e))R_j^e} f_\gamma](h) = f_\gamma\left(\{e^{t\sigma(S,e)n^j(b(e))\tau_j} h_e\}_{e\in E(\gamma)}\right). \quad (155)$$

Thus, the $W_t^n(S)$ act on the cylindrical functions by left translations in their arguments. The commutator of the Weyl-operators is

$$W_t^n(S) W_{t'}^{n'}(S')\,(W_t^n(S))^{-1} = \exp\left(t' \sum_{[e]\in E(\gamma)} \left[\sum_{x\in S'-S} \sigma([S']_x,[e])n'^j(x)\delta^{jk}\right.\right. \quad (156)$$

$$\left.\left. + \sum_{x\in S\cap S'} \sigma([S']_x,[e])n'^j(x)\left[e^{t\sigma([S']_x,[e])\mathrm{ad}_n(x)}\right]^{jk} R_k^{x,[e]}\right]\right),$$

where the calculation was performed in terms of germ operators [99] and we will not introduce them here. The important thing to see here is that the algebra between the Weyl-operators $W_t^n(S)$ does not close. However, the elements are explicitly calculable. After the substitution of the unbounded elements $a \in \mathfrak{P}$ by its associated Weyl functions $W_t(a)$ in the abstract quantum Lie *-algebra $\mathfrak{Q}$ we see that the elements of the quantum Lie *-algebra $\mathfrak{Q}$ are invertible and $\mathfrak{Q}$ is ***unital***, i.e. there exists a unique unit element. From this we can conclude that any representation of the quantum Lie *-algebra will be non-degenerate, that is for a representation π of $\mathfrak{Q}$ the identity $\pi(a)\psi = 0$ for all $a \in \mathfrak{Q}$ implies that $\mathcal{H} \ni \psi = 0$. Moreover, in any representation our generating elements are unitary which means they will become ***bounded operators***. We are in a situation where we can apply the following lemma, compare Lemma 8.1.1 in [9] and the proof therein or [100].

Lemma [100]: Sum of Cyclic Representations 2.2.2. *Every non-degenerate representation of the generators of a *-algebra by bounded operators is a direct sum of cyclic representations.*

So the basic building blocks of our representation for $\mathfrak{Q}$ will be ***cyclic representations***.

Definition [101]: Cyclic Representation 2.2.3. *A representation $(\mathcal{H}, \pi)$ of a *-algebra $\mathfrak{A}$ is said to be **cyclic** if there exists a normed vector $\Omega \in \mathcal{H}$ in the common domain of all $a \in \mathfrak{A}$ such that $\pi(\mathfrak{A})\Omega$ is dense in $\mathcal{H}$. Then the normed vector Ω is denoted as **cyclic vector**.*

To come to the cyclic representations, we need to go a few steps back. The classical gauge invariant configuration space $\mathcal{A}/\mathcal{G}$ consists of the space of smooth connections $\mathcal{A}$ modulo gauge transformations $\mathcal{G}$. For a quantization we will need to enlarge this space. We follow the presentation given in [102]. As a subalgebra we consider the ***holonomy algebra*** $\mathcal{HA}$ which is generated by finite linear combinations of holonomies on $\mathcal{A}/\mathcal{G}$ with complex coefficients. Since by construction it is closed under complex conjugation, which then is the involution operation, it is a *-subalgebra of the algebra of complex-valued, continuous bounded functions on $\mathcal{A}/\mathcal{G}$. We can complete $\mathcal{HA}$ with respect to the supremum norm

$$||f|| = \sup_{[A]\in\mathcal{A}/\mathcal{G}} |f([a])|, \quad (157)$$

where f is a continuous bounded function on $\mathcal{A}/\mathcal{G}$. The completition of $\mathcal{HA}$ with respect to this norm will be denoted by $\overline{\mathcal{HA}}$ and is a commutative C*-algebra. A ***C*-algebra*** $\mathfrak{A}$ is a Banach algebra with an involution, satisfying $||a^*a|| = ||a||^2$ for every $a \in \mathfrak{A}$. $\overline{\mathcal{HA}}$ has also an unique identity element $h_e(0,0)$ which means that the algebra is unital. Now we can make use of many powerful theorems introduced by ***Gelfand*** and ***Naimark*** concerning C*-algebras and their representations. Though first, let us introduce a few expressions. By the ***spectrum*** $\triangle(\mathfrak{A})$ of a unital Banach algebra $\mathfrak{A}$ we mean the set of all non-zero *-homomorphisms $\chi : \mathfrak{A} \to \mathbb{C}$; $a \mapsto \chi(a)$, called ***characters***, into the *-algebra of complex numbers. We denote the spectrum of $\overline{\mathcal{HA}}$ by $\overline{\mathcal{A}/\mathcal{G}}$. The classical configuration space of gauge invariant connections $\mathcal{A}/\mathcal{G}$ is densly embedded in $\overline{\mathcal{A}/\mathcal{G}}$. Next we define the ***Gelfand transform (representation)*** which is the map from the unital Banach algebra $\mathfrak{A}$ to all continuous linear functions $C^0(\triangle(\mathfrak{A}))$ on $\triangle(\mathfrak{A})$

$$\bigvee : \mathfrak{A} \to C^0(\triangle(\mathfrak{A})); \quad a \mapsto \check{a}, \text{ with } \check{a} := \chi(a). \tag{158}$$

Theorem [101]: Isometric Isomorphism 2.2.4. *Let $\mathfrak{A}$ be a unital, commutative C*-algebra. Then the Gelfand transform is an isometric ($||\check{a}|| = ||a||$) isomorphism between $\mathfrak{A}$ and the space of continuous functions on its spectrum.*

So $\overline{\mathcal{HA}}$ is isomorphic to the C*-algebra $C^0(\overline{\mathcal{A}/\mathcal{G}})$ of continuous functions on $\overline{\mathcal{A}/\mathcal{G}}$. Furthermore, one can show that the spectrum is a compact Hausdorff space.

Instead of the space $\overline{\mathcal{A}/\mathcal{G}}$ one often considers the space of ***generalized connections*** $\bar{\mathcal{A}}$ and let act the group of ***generalized gauge transformations*** $\bar{\mathcal{G}}$ on $\bar{\mathcal{A}}$ later on. Using the framework of projective techniques, see [102, 103], it can be shown that the spaces $\overline{\mathcal{A}/\mathcal{G}}$ and $\bar{\mathcal{A}}/\bar{\mathcal{G}}$ are isomorphic.

Definition [102]: Generalized connections $\bar{\mathcal{A}}$ 2.2.5. *The space of generalized or distributional connections $\bar{\mathcal{A}}$ on γ is the space of all maps $h_e : E(\gamma) \to G$ from the edges $E(\gamma)$ of a graph γ into the compact Hausdorff (topological) group G that satisfy*

1. $h_{e^{-1}} = h_e^{-1}$
2. $h(e_1 \circ e_2) = h(e_1)h(e_2)$.

*It can be shown that the generalized connections $\bar{\mathcal{A}}$ form a compact Hausdorff space in the so-called **Tychonoff topology** [9, 104].*

Notice that $\bar{\mathcal{A}}$ contains elements which are nowhere continuous (distributional). The generalized gauge transformations $\bar{\mathcal{G}}$ are the set of all maps $g : \sigma \to \mathrm{SU}(2)$, that is $\bar{\mathcal{G}} := \times_{x\in\sigma}\mathrm{SU}(2)$.

We are interested in finding a representation for $\overline{\mathcal{HA}}$. What we will use in the upcoming is that there is a two way relation between cyclic representations and ***positive linear functionals*** which are in algebraic terms referred to as ***states***. Namely, given a cyclic representation $(\pi, \mathcal{H}, \Omega)$ we can construct a state on $\mathfrak{Q}$ for $a \in \mathfrak{Q}$ by $\omega(a) := \langle \Omega, \pi(a)\Omega\rangle_{\mathcal{H}}$ and vice versa given a state on a *-algebra we can construct a unique, up to unitary equivalence, cyclic representation $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$ via the ***GNS construction***.

Theorem [101, 105]: GNS (Gelfand-Naimark-Segal) construction 2.2.6. *Let ω be a state on a unital *-algebra $\mathfrak{A}$. Then there exist a Hilbert space $\mathcal{H}_\omega$, a cyclic representation π_ω of $\mathfrak{A}$ on $\mathcal{H}_\omega$ and a normed cyclic vector $\Omega_\omega \in \mathcal{H}_\omega$, shortly denoted as GNS data $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$, such that*

$$\omega(a) := \langle \Omega_\omega, \pi_\omega(a)\Omega_\omega\rangle_{\mathcal{H}_\omega}. \tag{159}$$

Additionally, the GNS data is determined by eq. (159) uniquely up to unitary equivalence.

Due to the isomorphism between $\overline{\mathcal{HA}}$ and $C^0(\overline{\mathcal{A}/\mathcal{G}})$ the state $\omega(a)$ is also a positive linear functional on $C^0(\overline{\mathcal{A}/\mathcal{G}})$. Now our task is to find a suitable state $\omega(a)$ in order to be able to construct a cyclic representation for $\overline{\mathcal{HA}}$.

Theorem [104]: Riez-Markov 2.2.7. *Let X be a locally compact Hausdorff space and let $\omega : C^0(X) \to \mathbb{C}$ be a positive linear functional (state) on the space of continuous functions on X with $\omega(1) = 1$. Then there exists a unique, regular, Borel probability measure μ on the natural Borel σ-algebra $\mathfrak{A}$ of X, such that μ represents ω, that is,*

$$\omega = \int\limits_X \mathrm{d}\mu(x)\tilde{f}(x) \tag{160}$$

for all $\tilde{f} \in C^0(X)$.

In our case the state corresponding to $a \in \overline{\mathcal{HA}}$ is

$$\omega(a) = \int\limits_{\overline{\mathcal{A}/\mathcal{G}}} \mathrm{d}\mu([A])\tilde{f}([A]) \quad \text{or} \quad \omega(a) = \int\limits_{\overline{\mathcal{A}}} \mathrm{d}\mu(A)\tilde{f}(A) \tag{161}$$

for all $\tilde{f} \in C^0(\overline{\mathcal{A}/\mathcal{G}})$ and here the square brackets denote equivalence classes with respect to the gauge transformations, alternatively $\tilde{f} \in C^0(\overline{\mathcal{A}})$.

Since we know that the holonomies are elements of SU(2) and SU(2) is a compact gauge group, there exists a unique gauge-invariant and normalized measure, the so-called ***Haar measure***.

Definition [96]: Haar measure 2.2.8. *A left (right) invariant Haar measure μ_H^ℓ (μ_H^r) on a locally compact group G is a positive measure on G satisfying $\mu_H^\ell \circ \lambda_g^{-1} = \mu_H^\ell$ ($\mu_H^r \circ \rho_g^{-1} = \mu_H^r$) with left λ_g and right ρ_g translations as defined in 2.1.3 which is equivalent to*

$$\int\limits_G \mathrm{d}\mu_H^{\ell/r}(h)f(h) = \int\limits_G \mathrm{d}\mu_H^{\ell/r}(h)\begin{cases} f(gh) \\ f(hg) \end{cases} \quad \forall g, h \in G. \tag{162}$$

Theorem [96, 106]: Existence Haar measure 2.2.9. *For a finite dimensional Lie group G left μ_H^ℓ and right μ_H^r Haar measure exist and are unique up to positive constants. If G is compact, both measures are equal, i.e. $\mu_H^\ell = \mu_H^r$. They are unique if fixed to be probability measures (normalized). In this case the resulting Haar measure is also invariant under inversions, i.e. maps $h \mapsto h^{-1}$.*

With the help of the Haar measure we can define a scalar product which enables us to turn the space of functions cylindrical over a graph γ Cyl_γinto a Hilbert space. For $f, f' \in \mathrm{Cyl}_\gamma$ with respect to the *same* graph γ and ℓ copies of the Haar measure the scalar product is given by

$$\langle f|f'\rangle = \langle p_\gamma^* f_\gamma | p_\gamma^* f'_\gamma\rangle := \int\limits_{G^{|E(\gamma)|}} \prod_{e\in E(\gamma)} \mathrm{d}\mu_H(h_e)\, \overline{f\left(h_{e_1}[A], \ldots, h_{e_\ell}[A]\right)} f'\left(h_{e_1}[A], \ldots, h_{e_\ell}[A]\right). \tag{163}$$

This gives rise to a Hilbert space $\mathcal{H}_\gamma = \overline{\mathrm{Cyl}_\gamma}^{||\cdot||}$ associated with a graph γ and $\mathcal{H}_\gamma$ is isomorphic to $L_2(\mathrm{SU}(2)^\ell, \mathrm{d}\mu_H)$. Let from now on denote $\mathcal{H}_0$ the ***space of all cylindrical functions***. The form of $\mathcal{H}_\gamma$ and scalar product on $\mathcal{H}_\gamma$ guide us how $\mathcal{H}_0$ can be express as a space of square integrable functions and how we can construct a scalar product to turn $\mathcal{H}_0$ into a Hilbert space.

This brings us back to the question of finding a suitable measure on $\mathcal{H}_0$ and thus according to the Riez-Markov theorem a state. To reduce the infinite number of possible states on *-algebras one makes additional physically motivated assumptions such as that the representations should be ***irreducible*** and ***weakly continous***.

Definition [104]: Weakly and Strongly Continous 2.2.10. *A unitary operator $\hat{U}(a) := \pi(W(a))$, that is a unitary representation of an element of the algebra on a Hilbert space $\mathcal{H}$, is said to be **weakly continuous**, if for a one-parameter group of unitary operators $\hat{U}_t(a) := \pi(W_t(a))$ we have*

$$\lim_{t\to 0}\langle \psi, \hat{U}_t(a)\psi'\rangle = \langle \psi, \psi'\rangle, \tag{164}$$

*for all elements ψ, ψ' in $\mathcal{H}$. If in addition the one-parameter group of unitary operators satisfies $\hat{U}_{t+s}(a) = \hat{U}_t(a)\hat{U}_s(a)$ for all t, s in $\mathbb{R}$ it is called **strongly continuous**. Notice that for unitary operators weak continuity and strong continuity are equivalent.*

Due to Stone's theorem 2.2.11 this is important to see whether the operators of $\hat{a} := \pi(a)$ corresponding to the infinitesimal transformations caused by a exist or not.

Theorem [104]: Stone's Theorem 2.2.11. *Let $\hat{U}_t(a)$ be a strongly continous one-parameter group of unitary operators on a Hilbert space $\mathcal{H}$. Then there is a self-adjoint operator $\hat{a}$ on $\mathcal{H}$, called the **infinitesimal generator** of the group, such that $\hat{U}_t(a) = e^{it\hat{a}}$.*

With the definition of the so-called ***Ashtekar-Lewandowski Measure***, we obtain a measure that respects the supposed properties of the representations and with which we can define a scalar product such that we finally obtain a Hilbert space $\mathcal{H}_0$ for all cylindrical functions.

Definition [107]: Ashtekar-Lewandowski Measure 2.2.12. *Let $f = p^*_\gamma f_\gamma$ be a cylindrical function over a graph γ with the continuous complex valued function $f_\gamma : G^{|E(\gamma)|} \to \mathbb{C}$ acting on $|E(\gamma)|$ copies of a compact group G. We define the regular Borel probability measure on the generalized connections $\bar{\mathcal{A}}$, referred to as **Ashtekar-Lewandowski measure** μ_0, by*

$$\mu_0(f) := \mu_0(p^*_\gamma f_\gamma) = \int\limits_{G^{|E(\gamma)|}} \prod_{e\in E(\gamma)} \mathrm{d}\mu_H(h_e)\, f_\gamma(\{h_e\}_{e\in E(\gamma)}), \tag{165}$$

where μ_H is the Haar measure on the ℓ-th copy of G which is due to the compactness of G invariant under left and right translations as well as inversions. In LQG we have $G = \mathrm{SU}(2)$.

Our Hilbert space is then given by the space of μ_0 square integrable functions over generalized connections, that is

$$\mathcal{H}_0 = L_2\left(\bar{\mathcal{A}}, \mathrm{d}\mu_0\right). \tag{166}$$

The Hilbert space $\mathcal{H}_0$ is also the kinematical representation space we are looking for. It is convenient to introduce an orthonormal basis for $\mathcal{H}_0$. For the group $G = \mathrm{SU}(2)$ we can relate the construction of representations for holonomies over graphs γ with edges e to the construction of a representation for the angular momentum in quantum mechanics, see for example [108]. For SU(2) the edges of a graph and the irreducible representations, in correspondence to them, are labeled by half-integer spin quantum numbers $j_e = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$. Furthermore, we consider magnetic quantum numbers n_e, $m_e \in \{-j_e, -j_e+1, \ldots, j_e-1, j_e\}$ and then label the $(2j_e+1)$ dimensional irreducible representation related to an edge e by $[\pi(h_e)]_{j_e m_e n_e}$ and h_e is the holonomy along the edge e. One can show that these matrix elements can explicitly be written in terms of complex numbers $a, b, c, d \in \mathbb{C}$, see [9], by

$$[\pi(h_e)]_{j_e m_e n_e} = \sum_{\ell_e} \frac{\sqrt{(j_e+m_e)!(j_e-m_e)!(j_e+n_e)!(j_e-n_e)!}}{(j_e+n_e-\ell_e)!(m_e-n_e+\ell_e)!(j_e-m_e-\ell_e)!\ell_e!} a^{j_e+n_e-\ell_e} b^{m_e-n_e+\ell_e} c^{\ell_e} d^{j_e-m_e-\ell_e}, \tag{167}$$

where ℓ_e runs over all non-negative integers such that the factorials have non-negative arguments. Notice that the matrix elements have the same form for $G = \mathrm{SL}(2, \mathbb{C})$.

To make the connection with angular momentum in quantum mechanics we define the states

$$b_{j_e m_e m'_e}(h_e) := \langle h_e | j_e m_e \rangle_{m'_e} := \sqrt{2j_e + 1}\,[\pi(h_e)]_{j_e m_e m'_e}\,. \tag{168}$$

They constitute an orthonormal basis for the Hilbert space $L_2(\mathrm{SU}(2), \mathrm{d}\mu_H)$ according to the ***Peter & Weyl theorem*** for general compact gauge groups G.

Theorem [109, 110]: Peter & Weyl 2.2.13. *Let j be a labeling of the equivalence classes of finite dimensional irreducible representations of a compact Lie group G. Pick for each j a representative $(\pi_j, \mathcal{H}_j)$ and define*

$$b_{jmn}(g) := \sqrt{d_j}\,[\pi(g)]_{jmn} \tag{169}$$

with $m, n \in \{1, \ldots, d_j\}$, $d_j = dim(\mathcal{H}_j)$. The b_{jmn} form an orthonormal basis of the Hilbert space $\mathcal{H} = L_2(G, \mathrm{d}\mu_H)$, where μ_H is the Haar measure on G.

In quantum mechanics the angular momentum eigenstates for the angular momentum operator J_k in the spin j representation are given by $|jm\rangle$. They also form an orthonormal basis. The angular momentum operators J_k satisfy the algebra $[J_k, J_\ell] = i\epsilon_{k\ell p} J_p$. For the states $|j_e m_e\rangle_{m'_e}$ the action of the right-invariant vector fields R^e_k is given by

$$R^e_k |j_e m_e\rangle_{m'_e} = \frac{d}{dt}|_{t=0}\, U(\exp(t\tau_k))|j_e m_e\rangle_{m'_e} \tag{170}$$

with $\tau_k = -i\sigma_k$ and σ_k, $k = 1, 2, 3$ are the Pauli matrices. In case we define $Y_k := -iR^e_k/2$, the Y_k satisfy the algebra $[Y_k, Y_\ell] = i\epsilon_{k\ell p} Y_p$ which is exactly the same as for the J_k. From this we can conclude that for fixed m'_e there exists a unitary transformation between the Hilbert spaces $\mathcal{H}^{j_e}_{m'_e}$ spanned by the sates $|j_e m_e\rangle_{m'_e}$ and $\mathcal{H}^j$ spanned by the states $|jm\rangle$.

Next we can generalize the definition of the state for single edges e to graphs γ with arbitrary but finitely many edges. Therefore, we define the ***spin network functions*** $T_{\gamma\vec{j}\vec{m}\vec{n}}$ which provide an orthonormal basis for the Hilbert space $\mathcal{H}_0 = L_2\big(\bar{\mathcal{A}}, \mathrm{d}\mu_0\big)$.

Definition [9]: Spin Network Function 2.2.14. *For a graph γ with finitely many edges e the spin network functions are the maps $T_{\gamma\vec{j}\vec{m}\vec{n}} : \bar{\mathcal{A}} \to \mathbb{C}$, $h = \{h\}_{e\in E(\gamma)} \mapsto T_{\gamma\vec{j}\vec{m}\vec{n}}(h)$, explicitly written as*

$$T_{\gamma\vec{j}\vec{m}\vec{n}}(h) := \prod_{e\in E(\gamma)} b_{j_e m_e n_e}(h_e) = \prod_{e\in E(\gamma)} \sqrt{2j_e + 1}\,[\pi(h_e)]_{j_e m_e n_e} \tag{171}$$

with $\vec{j} = \{j_e\}_{e\in E(\gamma)}$, $\vec{m} = \{m_e\}_{e\in E(\gamma)}$ and $\vec{n} = \{n_e\}_{e\in E(\gamma)}$.

The spin network functions $T_{\gamma\vec{j}\vec{m}\vec{n}}$ satisfy the following properties:

1. They form an orthonormal basis of the Hilbert space $\mathcal{H}_0$, i.e.

$$\langle T_{\gamma\vec{j}\vec{m}\vec{n}}, T_{\gamma'\vec{j}'\vec{m}'\vec{n}'}\rangle = \int \mathrm{d}\mu_0\, \overline{T_{\gamma\vec{j}\vec{m}\vec{n}}} T_{\gamma'\vec{j}'\vec{m}'\vec{n}'} = \delta_{\gamma\gamma'}\delta_{jj'}\delta_{mm'}\delta_{nn'}. \tag{172}$$

2. The span of the $T_{\gamma\vec{j}\vec{m}\vec{n}}$ is dense in $\mathcal{H}_0$.

According to the Riez-Markov theorem the state we are looking for is given by $\omega_0(f) = \mu_0(f)$ for $f \in \mathrm{Cyl}$. The vector fields $Y_n(S)$ can also be incooperated in the definition of the state which leads to the so-called ***Ashtekar(-Isham)-Lewandowski state*** which is precisely given as

Theorem [95, 107, 111]: Ashtekar(-Isham)-Lewandowski State 2.2.15. *The only diffeomorphism invariant state on the holonomy-flux algebra $\mathfrak{P}$, respectively $\mathfrak{Q}$, is the so-called Ashtekar(-Isham)-Lewandowski state ω_0:*

$$\omega_0(fY_{n_1}(S_1)\dots Y_{n_N}(S_N)) := \begin{cases} 0, & N > 0 \\ \mu_0(f) \end{cases} \tag{173}$$

Then the GNS construction tells us that there exists a cyclic representation π_0 such that

$$\begin{aligned} \pi_0(f) \cdot \psi &:= f[h_e]\psi, \\ \pi_0(W^n_t(S)) \cdot \psi &:= W^n_t(S)[\psi] \end{aligned} \tag{174}$$

More modern considerations about the Ashtekar(-Isham)-Lewandowski state and alternative vacuum states for LQG can for instance be found in [112] and [113].

Let us summarize the main results:

Theorem [9]: Existence 2.2.16. *The kinematical LQG Hilbert space is the space of square integrable functions over* ***generalized connections*** *$\bar{\mathcal{A}}$, see definition 2.2.5, with respect to the* ***uniform measure*** *μ_0*

$$\mathcal{H}_0 = L_2\left(\bar{\mathcal{A}}, \mathrm{d}\mu_0\right). \tag{175}$$

Let $\mathcal{D}$ be a dense subspace of $\mathcal{H}_0$ spanned by finite linear combinations of ***spin network functions (SNF)****, then we can find a representation π_0 of $\mathfrak{Q}$ such that the cylindrical functions f act by multiplication and the vector fields $W^n_t(S)$ act as derivations of $\psi \in \mathcal{D}$, that is*

$$\begin{aligned} \pi_0(f) \cdot \psi &= f\psi, \\ \pi_0(W^n_t(S)) \cdot \psi &= W^n_t(S)[\psi], \end{aligned} \tag{176}$$

*where $W^n_t(S)[\psi]$ denotes the action of the Weyl algebra element of a vector field on a $\psi \in \mathcal{D}$. Furthermore, the representations of f and $W^n_t(S)$ satisfy canonical commutation relations and the *relations.*

2.3 Volume Operator

Next we display the derivation of the volume operator, as defined in [114], on the kinematical Hilbert space $\mathcal{H}_0$ using a ***point-splitting regularization*** introduced in [115]. Aside to the definition of the volume operator in [114] there exists an alternative definition of the volume operator given in [116]. For kinematical and dynamical reasons explained in [9], we will however stick to the definition given in [114]. We display the regularization procedure following the presentation given in [9]. Later the volume operator will be used in the definition of the Hamiltonian constraint operator. Its quantization is also a guiding principle in the quantization of our physical Hamiltonian operator obtained from four modified Klein-Gordon scalar fields in section 9. However, we will not display the derivation of the area [117] and length operator here, which can be derived in a similar way, since we will not use them. For $D = 3$ and an open, connected region $R \in \sigma$ we define the ***volume functional*** by

$$\mathrm{V}(R) := \int_R \mathrm{d}^3x \sqrt{q}, \tag{177}$$

where we choose a coordinate system. We want to rewrite this expression in terms of densitized triads $E^a_j = \sqrt{q}e^a_j$. Recall that $q := \det(q_{ab})$ and $\sqrt{q} = \sqrt{|\det(E^a_j)|} = \det\big(e^j_a\big) \geq 0$. This yields to the identity

$$\det(E^a_j) = \frac{1}{3!}\epsilon^{ijk}\epsilon_{abc}E^a_i E^b_j E^c_k = \mathrm{sgn}\big(\det(E^a_j)\big)\, q \tag{178}$$

with this the volume functional becomes

$$\mathrm{V}(R) = \int_R \mathrm{d}^3x \sqrt{\left|\frac{1}{3!}\epsilon^{ijk}\epsilon_{abc}E^a_i E^b_j E^c_k\right|}, \tag{179}$$

where we have taken into account that classically $\det(E^a_j) > 0$. Let us introduce a so-called ***cubulation*** of R which means that we fill out the open region R by cubes. We choose an arbitrary but fixed coordinate frame. Let p be the centre of a cube $\square$, x be a coordinate point inside the cube and let $\vec{n}_i$ be the right-oriented normal vectors in the chosen frame. Then the cube is spanned by the three vectors $\vec{\square}_i = \square_i\vec{n}_i$ and the volume of the cube is given by $\mathrm{vol}(\square) = \square_1\square_2\square_3\det(\vec{n}_1, \vec{n}_2, \vec{n}_3)$. Let $\chi_\square(p, x)$ be the characteristic function corresponding to the coordinates of the cube, such that in the limit when we shrink the size of the cube to zero $\square \to 0$ the limit $\lim\limits_{\square\to 0}\frac{\chi_\square(p,x)}{\mathrm{vol}(\square)} = \delta^{(3)}(p, x)$ reassembles the delta distribution. We define the smeared quantity

$$\begin{aligned} E(p, \square, \square', \square'') := \frac{1}{\mathrm{vol}(\square)\mathrm{vol}(\square')\mathrm{vol}(\square'')} \int_\sigma \mathrm{d}^3x \int_\sigma \mathrm{d}^3y \int_\sigma \mathrm{d}^3z \\ \chi_\square(p, x)\, \chi_{\square'}(2p, x + y)\, \chi_\square(3p, x + y + z)\frac{1}{3!}\epsilon^{ijk}\epsilon_{abc}E^a_i(x)E^b_j(y)E^c_k(z). \end{aligned} \tag{180}$$

To visualize the situation, imagine three cubes in a row with coordinate centers at p, $2p$ and $3p$. Each center of a cube will later reassemble one vertex of an underlying graph. With the help of $E(p, \square, \square', \square'')$ we reproduce the volume functional in the limit when $\square, \square', \square'' \to 0$ shrink to zero evaluated at the point p, that is

$$V(R) = \lim_{\square\to 0}\lim_{\square'\to 0}\lim_{\square''\to 0}\int_R \mathrm{d}^3p \sqrt{\Big|E(p, \square, \square', \square'')\Big|}. \tag{181}$$

For the Poisson bracket convention $\{A^j_b(x), E^a_i(y)\} = -\frac{\kappa\beta}{2}\delta^a_b\delta^j_i\delta^{(3)}(x, y)$ we find that the operator corresponding to E^a_i can be expressed as a functional derivative by

$$\hat{E}^a_i(x) = i\frac{\ell_P^2}{2}\frac{\delta}{\delta A^i_a(x)}, \tag{182}$$

acting on functions of smooth connections $\mathcal{A}$. After performing the limits, i.e. removing the regulator, the action of the final volume operator can be generalized to functions on the space of generalized connections $\bar{\mathcal{A}}$.

The smeared and regularized version of the operator $\hat{E}^a_i(x)$ reads

$$\hat{E}^a_i(p, \square) := \frac{1}{\mathrm{vol}(\square)}\int_\sigma \mathrm{d}^3x\, \chi_\square(p, x)\hat{E}^a_i(x). \tag{183}$$

So as an ansatz for $\hat{E}(p,\square,\square',\square'')$ we get

$$\hat{E}(p,\square,\square',\square'') = \frac{1}{3!}\epsilon^{ijk}\epsilon_{abc}\hat{E}^a_i(p,\square)\hat{E}^b_k(2p,\square)\hat{E}^c_k(3p,\square). \tag{184}$$

Consider a graph γ and an edge $e \in E(\gamma)$ as a representative element from the set of edges of the graph γ. Let the edge e be restricted by the vertices $v, v' \in V(\gamma)$, which are beginning or ending points of the edge. We want every edge to be outgoing from a vertex v. If necessary, we can subdivide an edge e into segments $s\circ(s')^{-1}$, such that the segments s and s' are outgoing from the vertices v and v'. The so gained extra vertices $\tilde{v} = e\cap e'$ will not lead to additional contributions, when we construct the volume operator, since as we are going to see only the vertices $v = p$ will contribute. We parametrize the edge e by $e : [0,1] \to \sigma, t \mapsto \sigma(t)$. Next, consider the action of a single operator $\hat{E}^a_i(p,\square)$ on a cylindrical function on the graph γ $f = p^*_\gamma f_\gamma$, which leads to

$$\begin{aligned}
\hat{E}^a_i(p,\square)f(h_e[A]) &= \frac{1}{\mathrm{vol}(\square)}\int_\sigma \mathrm{d}^3x\, \chi_\square(p,x)\hat{E}^a_i(x)f_\gamma(h_e[A]) \\
&= \frac{i\ell_P^2}{2}\frac{1}{\mathrm{vol}(\square)}\int_\sigma \mathrm{d}^3x\, \chi_\square(p,x)\frac{\delta}{\delta A^i_a(x)}f_\gamma(h_e[A]) \\
&= \frac{i\ell_P^2}{2}\frac{1}{\mathrm{vol}(\square)}\int_\sigma \mathrm{d}^3x\, \chi_\square(p,x)\frac{\delta h_e}{\delta A^i_a(x)}\frac{\delta}{\delta h_e}f_\gamma(h_e[A]) \\
&= \frac{i\ell_P^2}{2}\frac{1}{\mathrm{vol}(\square)}\sum_{e\in E(\gamma)}\int_0^1 \mathrm{d}t\, \chi_\square(p,e(t))\dot{e}^a(t)\frac{1}{2}\mathrm{Tr}\left([h_e(0,t)\tau_i h_e(t,1)]\,\frac{\delta}{\delta h^T_e(0,1)}\right)f_\gamma
\end{aligned} \tag{185}$$

with $\tau_j := -i\sigma_j$ and σ_j, $j = 1,2,3$ are the Pauli matrices. Here we write $f = f(h_e[A])$ to explicitly display the dependence of the cylindrical function on the holonomies and the dependence of the holonomies on the connections. The action of the operator $\hat{E}(p,\square,\square',\square'')$ will contain three types of terms: a term that arises from the action of three functional derivatives on a cylindrical function f_γ. Terms from letting one functional derivative act on a $\hat{E}(p,\square)$ and two functional derivatives acting on f_γ and terms coming from the action of two functional derivative on $\hat{E}(p,\square)$ and one functional derivative acting on f_γ. We mention here that only the term where all three functional derivatives act on f_γ survives due to the vanishing contractions of ϵ^{ijk} with terms containing traces of $\tau_i\tau_j + \tau_j\tau_i$, $\tau_j\tau_k + \tau_j\tau_k$ and $\tau_k\tau_i + \tau_i\tau_k$, for details see [9]. Therefore, we are left with

$$\hat{E}(p,\square,\square',\square'')f = \frac{1}{3!}\epsilon^{ijk}\epsilon_{abc}\hat{E}^a_i(p,\square)\hat{E}^b_k(2p,\square)\hat{E}^c_k(3p,\square)f_\gamma \tag{186}$$

$$\begin{aligned}
&= \frac{-i\ell_P^6}{8}\frac{1}{8\cdot 3!}\frac{1}{\mathrm{vol}(\square)\mathrm{vol}(\square')\mathrm{vol}(\square'')}\int_0^1 \mathrm{d}t\int_0^1 \mathrm{d}t'\int_0^1 \mathrm{d}t'' \\
&\Bigg\{\sum_{e,e',e''\in E(\gamma)}\epsilon^{ijk}\epsilon_{abc}\dot{e}^a(t)\dot{e}'^b(t')\dot{e}''^c(t'') \\
&\chi_\square(p,e(t))\,\chi_{\square'}(2p,e(t)+e'(t'))\,\chi_{\square''}(3p,e(t)+e'(t')+e''(t'')) \\
&\mathrm{Tr}\left([h_{e''}(0,t'')\tau_i h_{e''}(t'',1)]\,\frac{\delta}{\delta h^T_e(0,1)}\right)\mathrm{Tr}\left([h_{e'}(0,t')\tau_j h_{e'}(t',1)]\,\frac{\delta}{\delta h^T_e(0,1)}\right) \\
&\mathrm{Tr}\left([h_e(0,t)\tau_k h_e(t,1)]\,\frac{\delta}{\delta h^T_e(0,1)}\right)\Bigg\}f_\gamma.
\end{aligned} \tag{187}$$

One defines a function of edges e, e', e'' of a graph γ by $x_{ee'e''}(t,t',t'') := e(t) + e'(t') + e''(t'')$ and observes that its Jacobi determinant is equal to

$$\det\left(\frac{\partial\left(x_{ee'e''}\right)(t,t',t'')}{\partial(t,t',t'')}\right) := \det\left(\frac{\partial\left(x^1_{ee'e''}, x^2_{ee'e''}, x^3_{ee'e''}\right)(t,t',t'')}{\partial(t,t',t'')}\right) = \epsilon_{abc}\dot{e}^a(t)\dot{e}'^b(t')\dot{e}''^c(t'') \tag{188}$$

which reproduces the product of derivatives of the edges with respect to the parameter t entering the integral. The integral will vanish, if the Jacobi determinant is equal to zero or if not all edges e, e', e'' intersect in one common point p. The last point is due to the characteristic functions $\chi_\square$ which have their support in a neighbourhood around p whose size is determined by the size of the $\square_i$. In case that even one of the edges does not intersect the other two edges in p and we shrink the $\square_i$ to some small enough finite size $\square_0$, the characteristic function $\chi_\square$ will vanish. Therefore, let us assume that all of the three edges e, e', e'' intersect in a point p at unique parameter values t_0, t'_0, t''_0, where the uniqueness is guaranteed by the fact that the edges are not self-intersecting. The edges can be parametrized by

$$e(t) = p + c(t - t_0), \quad e'(t') = p + c'(t' - t'_0), \quad e''(t'') = p + c''(t'' - t''_0) \tag{189}$$

for analytic functions c, c', c'' vanishing at $t - t_0 = 0$ or $t' - t'_0 = 0$, $t'' - t''_0 = 0$ respectively.

First we take the limit $\lim\limits_{\square''\to 0} \frac{\chi_{\square''}(3p, e(t)+e'(t')+e''(t''))}{\mathrm{vol}(\square')} = \delta^{(3)}(3p, x_{ee'e''})$ leading to

$$\lim_{\square''\to 0} \hat{E}(p,\square,\square',\square'')f = \frac{-i\ell_P^6}{8}\frac{1}{8\cdot 3!}\frac{1}{\mathrm{vol}(\square)\mathrm{vol}(\square')}\int_0^1 \mathrm{d}t \int_0^1 \mathrm{d}t' \int_0^1 \mathrm{d}t'' \tag{190}$$

$$\Bigg\{\sum_{e,e',e''\in E(\gamma)} \epsilon^{ijk}\det\left(\frac{\partial\left(x_{ee'e''}\right)(t,t',t'')}{\partial(t,t',t'')}\right)$$
$$\chi_\square(p, e(t))\,\chi_{\square'}(p, e(t)+e'(t'))\,\delta^{(3)}(3p, x_{ee'e''})$$
$$\mathrm{Tr}\left([h_{e''}(0,t'')\tau_i h_{e''}(t'',1)]\,\frac{\delta}{\delta h_e^T(0,1)}\right)\mathrm{Tr}\left([h_{e'}(0,t')\tau_j h_{e'}(t',1)]\,\frac{\delta}{\delta h_e^T(0,1)}\right)$$
$$\mathrm{Tr}\left([h_e(0,t)\tau_k h_e(t,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\right)\Bigg\} f_\gamma. \tag{191}$$

We concentrate on the cases for which the Jacobi determinant is not equal to zero, i.e. $\det\left(\frac{\partial(x_{ee'e''})(t,t',t'')}{\partial(t,t',t'')}\right) \neq 0$. Then the function $x_{ee'e''}(t,t',t'')$ is invertible in a neighbourhood of p and its value at the point (t,t',t'') is $x_{ee'e''}(t_0,t'_0,t''_0) = 3p$. Since we chose the edges to be outgoing from a vertex v, it follows that the intersection point p has to be equal to the common vertex v of the edges, i.e. $p = v = e \cap e' \cap e''$, to lead to a non-vanishing result. In our parametrization the vertex is equal to $v = e(0) = e'(0) = e''(0)$, so we need to set $t = t' = t'' = 0$ and $t_0 = t'_0 = t''_0 = 0$ to reach at the vertex v. As a consequence we can replace the characteristic functions $\chi_\square(p, e(0)), \chi_{\square'}(2p, e(0)+e'(0))$ by $\chi_\square(p, v)$ and $\chi_{\square'}(p, v)$ which gives

$$\lim_{\square''\to 0}\hat{E}(p,\square,\square',\square'')f = \frac{-i\ell_P^6}{8}\frac{1}{8\cdot 3!}\frac{1}{\mathrm{vol}(\square)\mathrm{vol}(\square')}\int_0^1 \mathrm{d}t\int_0^1 \mathrm{d}t'\int_0^1 \mathrm{d}t'' \tag{192}$$

$$\Bigg\{\sum_{e,e',e''\in E(\gamma)}\epsilon^{ijk}\det\left(\frac{\partial\left(x_{ee'e''}\right)(t,t',t'')}{\partial(t,t',t'')}\right)\chi_\square(p,v)\,\chi_{\square'}(p,v)\,\delta^{(3)}(3p,x_{ee'e''})$$
$$\mathrm{Tr}\Bigg([h_{e''}(0,t'')\tau_i h_{e''}(t'',1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Bigg)\,\mathrm{Tr}\Bigg([h_{e'}(0,t')\tau_j h_{e'}(t',1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Bigg)$$
$$\mathrm{Tr}\Bigg([h_e(0,t)\tau_k h_e(t,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Bigg)\Bigg\}f_\gamma. \tag{193}$$

We approximate the integrals over t,t',t'' by

$$\int_0^1 \mathrm{d}t\int_0^1 \mathrm{d}t'\int_0^1 \mathrm{d}t''\,\det\left(\frac{\partial\left(x_{ee'e''}\right)(t,t',t'')}{\partial(t,t',t'')}\right)\delta^{(3)}(3p,x_{ee'e''}) \tag{194}$$
$$=\epsilon(e,e',e'')\left(\frac{1}{2}\right)^3\int_{\mathbb{R}}\mathrm{d}x^3\delta^{(3)}(p,x)=\frac{1}{8}\epsilon(e,e',e''),$$

where we defined

$$\epsilon(e,e',e''):=\epsilon_{abc}\dot{e}^a(0)\dot{e}'^b(0)\dot{e}''^c(0)=\mathrm{sgn}\left(\det(\dot{e}(0),\dot{e}'(0),\dot{e}''(0))\right). \tag{195}$$

Alternatively to sending $\square''\to 0$ first, we could have expanded the t,t',t''-integrals of functions $h(t)$, $g(t')$ and $\ell(t'')$, representing the corresponding functions in the integral, around $t=t'=t''=0$ in a small parameter ϵ corresponding to the length of an edge of a cube, resulting in

$$\int_0^1 \mathrm{d}t\int_0^1 \mathrm{d}t'\int_0^1 \mathrm{d}t''\,\ell(t'')g(t')h(t)f_\gamma \tag{196}$$
$$=\left(\ell(0)g(0)h(0)\int_0^{\epsilon/2}\mathrm{d}t\int_0^{\epsilon/2}\mathrm{d}t'\int_0^{\epsilon/2}\mathrm{d}t''+o(\epsilon^3)\right)f_\gamma=\left(\frac{\epsilon^3}{8}\ell(0)g(0)h(0)+o(\epsilon^3)\right)f_\gamma.$$

We will also use this technique in part III in section 9 to derive our physical Hamiltonian operator. So in the limes $\square''\to 0$ the regularized operator becomes

$$\lim_{\square''\to 0}\hat{E}(p,\square,\square',\square'')f = \frac{-i\ell_P^6}{8}\frac{1}{8\cdot 3!}\frac{1}{\mathrm{vol}(\square)\mathrm{vol}(\square')} \tag{197}$$
$$\Bigg\{\sum_{e,e',e''\in E(\gamma)}\frac{1}{8}\epsilon^{ijk}\det\left(\frac{\partial\left(x_{ee'e''}\right)(t,t',t'')}{\partial(t,t',t'')}\right)\chi_\square(p,v)\,\chi_{\square'}(p,v)$$
$$\mathrm{Tr}\Bigg([\tau_i h_{e''}(0,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Bigg)\,\mathrm{Tr}\Bigg([\tau_j h_{e'}(0,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Bigg)\,\mathrm{Tr}\Bigg([\tau_k h_e(0,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Bigg)\Bigg\}f_\gamma,$$

where we used that $h_{e''}(0,0)=h_{e'}(0,0)=h_e(0,0)=\hat{\mathbb{1}}$ and the ϵ^3 from the expansion of the integral cancels against $\frac{1}{\mathrm{vol}(\square'')}=\frac{1}{\epsilon^3}$. We introduce the right invariant vector fields

$$X_i^e:=\mathrm{Tr}\Bigg([\tau_i h_{e''}(0,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Bigg). \tag{198}$$

With these replacements and definitions we have

$$\lim_{\Box''\to 0}\hat{E}(p,\Box,\Box',\Box'')f = \frac{-i\ell_P^6}{8}\frac{1}{8\cdot 3!}\frac{1}{\mathrm{vol}(\Box)\mathrm{vol}(\Box')} \left\{\sum_{e,e',e''\in E(\gamma)}\frac{1}{8}\epsilon^{ijk}\epsilon_{abc}\dot{e}^a(0)\dot{e}'^b(0)\dot{e}''^c(0)\,\chi_\Box(p,v)\,\chi_{\Box'}(p,v)\,X_i^e X_j^{e'} X_k^{e''}\right\}f_\gamma. \tag{199}$$

Next we identify $\Box' = \Box$ which yields to

$$\lim_{\Box''\to 0}\hat{E}(p,\Box,\Box',\Box'')f = \frac{-i\ell_P^6}{8^2}\frac{1}{8\cdot 3!}\frac{\chi_\Box^2(p,v)}{(\mathrm{vol}(\Box))^2}\left\{\sum_{e,e',e''\in E(\gamma)}\epsilon(e,e',e'')\epsilon^{ijk}X_i^e X_j^{e'} X_k^{e''}\right\}f_\gamma \tag{200}$$

Finally, we substitute the sum over all triples of edges $\sum_{e,e',e''}$ incident at a common vertex v by a sum $\sum_{v\in V(\gamma)}$ over all vertices $v\in V(\gamma)$ followed by a sum $\sum_{e\cap e'\cap e''=v}$ over all triples incident at the same vertex v. We end up with the volume operator

$$\hat{V}(R)f_\gamma := \frac{\ell_p^3}{8}\sum_{v\in V(\gamma)\cap R}\sqrt{\left|\frac{i}{8\cdot 3!}\sum_{e\cap e'\cap \tilde{e}}\epsilon(e,e',e'')\epsilon^{ijk}X_i^e X_j^{e'} X_k^{e''}\right|}f_\gamma, \tag{201}$$

where the sum runs over the set $V(\gamma)$ of all vertices v of a graph γ. The volume operator is a linear unbounded operator on $\mathcal{H}_0$ which is symmetric, positive semidefinite and essentially self-adjoint (possible self-adjoint extensions). Its spectrum is discrete, for details on the spectrum see [115, 118, 119, 120, 121].

2.4 Dirac Quantization and Solutions of the Constraints

2.4.1 Gauß Constraint

By making the transition to the densitized triad E_j^a (electric field) and new connection A_a^j an additional constraint, the Gauß constraint, arose. Classically, the smeared version of the Gauß constraint is given by

$$G(\Lambda) = \int_\sigma \mathrm{d}^3x\Lambda^j G_j = \int_\sigma \mathrm{d}^3x\Lambda^j\left(\mathcal{D}_a E_j^a\right) = -\int_\sigma \mathrm{d}^3x\left(\mathcal{D}_a\Lambda^j\right)E_j^a = -E(\mathcal{D}\Lambda), \tag{202}$$

here the last equation follows from partial integration (no boundary). So in principle we have a densitized triad smeared in three dimensions and can apply a similar quantization procedure as in case of the holonomies and fluxes. In case of the holonomy and fluxes one needs to regularize both of them to calculate their Poisson bracket. The regularization procedure includes a three dimensional integral. Here to calculate the Poisson bracket one has only to regularize the holonomy h_e, since $G(\Lambda)$ already contains a three dimensional integral. We leave out the details of the regularization process, which can in detail be found in [9], and follow the lines of [12] to compute the expression for the Gauß constraint operator. After the regulator is removed, we are left with the Poisson bracket

$$\nu_{D\Lambda}(h_e) := \{G(\Lambda), h_e(A)\} = \beta\kappa\int_0^1 \mathrm{d}t\,\mathcal{D}_a\Lambda^j(e(t))\dot{e}^a(t)\,h_e(0,t)(A)\frac{\tau_j}{2}h_e(t,1)(A) \tag{203}$$

with $\mathcal{D}_a\Lambda^j = \partial_a\Lambda^j + f^j_{k\ell}A_a^k\Lambda^\ell$. Soon we will see that the expression under the integral can be written as the total time derivative of a product of holonomies. As a concrete basis for su(2) we choose $\tau_j = -i\sigma_j$ with σ_j, $j = 1, 2, 3$ being the Pauli matrices. In this case the structure constants $f_{jk\ell}$ are given by the totally skew symbol $\epsilon_{jk\ell}$. We set $\Lambda := \Lambda^j \tau_j$ and consider the term

$$\mathcal{D}_a \Lambda(e(t))\dot{e}^a(t) = \frac{d\Lambda}{dt} + \epsilon^j_{k\ell} A^k_a \Lambda^\ell \tau_j \dot{e}^a(t) = \frac{d\Lambda}{dt} + \frac{1}{2}\left[\tau_k, \tau_\ell\right] A^k_a \Lambda^\ell \dot{e}^a(t) = \frac{d\Lambda}{dt} + \left[A(e(t)), \Lambda\right], \quad (204)$$

where we used $[\tau_k, \tau_\ell] = 2\epsilon^j_{k\ell}\tau_j$ and we define $A(e(t)) := \dot{e}^a(t) A^j_a(e(t))\tau_j/2$. With this the term under the integral, hiding the arguments, reads

$$h_e(0,t)\left(\frac{d\Lambda}{dt} + [A(e(t)), \Lambda]\right) h_e(t,1). \quad (205)$$

Remember that the $h_e(0,t)(A)$ satisfy the parallel transport differential equation

$$\frac{d}{dt} h_e(0,t) = h_e(0,t) A(e(t)) \quad (206)$$

and the holonomy is defined as the unique solution $h_e(A) := h_e(0,1)$ with $h_e(0,0) = \mathbb{1}_{\mathrm{SU}(2)}$ thereof, compare definition 2.1.1. Furthermore, we can derive from the parallel transport equation that

$$\frac{d}{dt} h_e(t,1) = -A(e(t)) h_e(t,1) \quad (207)$$

and $h_e(1,1) = \mathbb{1}_{\mathrm{SU}(2)}$. Now applying the chain rule, with respect to the d/dt derivative, to the expression $h_e(0,t)\Lambda h_e(t,1)$ and inserting the derivatives of the individual terms we obtain

$$\frac{d}{dt}\left(h_e(0,t)\Lambda h_e(t,1)\right) = h_e(0,t)\left(\frac{d\Lambda}{dt} + [A(e(t)), \Lambda]\right) h_e(t,1). \quad (208)$$

This shows that the expression under the integral can indeed be written as a total derivative and consequently we obtain, after performing the integral,

$$\nu_{D\Lambda}(h_e) = \{G(\Lambda), h_e\} = -\frac{\beta\kappa}{2}\left(\Lambda(e(0)) h_e(A) - h_e(A)\Lambda(e(1))\right). \quad (209)$$

The generalization to cylindrical functions using the definitions of left and right invariant vector fields 2.1.3, compare eq. (144), leads to

$$\nu_{D\Lambda}(f) = \{G(\Lambda), f\} = -\frac{\beta\kappa}{4} \sum_{e \in E(\gamma)} \left(\Lambda^j(b(e)) R^e_j - \Lambda^j(f(e)) L^e_j\right) f_\gamma(A), \quad (210)$$

$$= -\frac{\beta\kappa}{4} \sum_{v \in V(\gamma)} \Lambda^j(v) \left[\sum_{e \in E(\gamma); v = b(e)} R^e_j - \sum_{e \in E(\gamma); v = f(e)} L^e_j\right] f_\gamma(A), \quad (211)$$

where the parametrization t of the edge is chosen such that $b(e) = e(0)$ is the beginning and $f(e) = e(1)$ is the final point of the edge and we finally expressed everything in terms of a sum over vertices of γ. We identify $G(\Lambda)[f] = -\nu_{D\Lambda}(f)$ which is real-valued, since Λ is real-valued for compact G.

Then the Gauß constraint operator is given by

$$\hat{G}(\Lambda)[f] = \frac{i\beta\ell_P^2}{4} \sum_{v \in V(\gamma)} \Lambda^j(v) \left[\sum_{e \in E(\gamma); v = b(e)} R^e_j - \sum_{e \in E(\gamma); v = f(e)} L^e_j\right] f_\gamma(A). \quad (212)$$

It is essentially self-adjoint with dense domain $C(\bar{\mathcal{A}})$, see for example [9].

Now we come to the ***solutions to the Gauß Constraint***. Notice that the Gauß constraint can be solved before or after solving the diffeomorphism or Hamiltonian constraint. Moreover, we can deal with the Gauß constraint in two different ways. We can solve the Gauß constraint on the classical level and work directly with gauge invariant states, as explained in section 2.2.2, or we can solve the Gauß constraint at the quantum level on $\mathcal{H}_0$ what we are about to do now following the lines of [11]. According to section 2.2.2 the kinematical LQG Hilbert space, i.e. without solving the constraints, is given by $\mathcal{H}_0 := L_2\left(\bar{\mathcal{A}}, \mathrm{d}\mu_0\right)$. Since the SU(2) Gauß constraint only arises due to the variable transformation to the new connection and densitized triad variables, we will nevertheless denote the Hilbert space after solving the Gauß constraint with $\mathcal{H}_{\text{kin}} = L_2\left(\overline{\mathcal{A}/\mathcal{G}}, \mathrm{d}\mu_0\right)$. Here we point out that $\mathcal{H}_{\text{kin}} \subset \mathcal{H}_0$, so $\mathcal{H}_{\text{kin}}$ is a subspace of $\mathcal{H}_0$. Recall from definition 2.1.1 that a holonomy transforms under SU(2) gauge transformations with $g \in \mathrm{SU}(2)$ as $h_e(A) \mapsto h_e^g(A) = g(b(e))h_e(A)g(f(e))^{-1}$, where $b(e) := e(0)$ and $f(e) := e(1)$ denote the beginning and the final point of an edge, which are the vertices of a graph. Notice that the gauge transformations only act on the vertices of a graph. Therefore, a gauge invariant cylindrical function should be invariant under the action of SU(2) at the beginning and final points of edges, i.e.

$$f_{\text{kin}}(h_{e_1}, \ldots, h_{e_n}) \stackrel{!}{=} f_{\text{kin}}(g(b(e_1))h_{e_1}(A)g(f(e_1))^{-1}, \ldots, g(b(e_n))h_{e_n}(A)g(f(e_n))^{-1}) \tag{213}$$

for $f_{\text{kin}} \in \mathcal{H}_{\text{kin}}$. We can reduce the problem of constructing gauge invariant cylindrical functions to the task of finding a gauge invariant basis in terms of spin network function, sometimes called ***spin network states***. We define the gauge variant spin network functions (SNF) as

$$T_{\gamma\vec{j}\vec{m}\vec{n}}(h) := \prod_{e\in E(\gamma)} b_{j_e m_e n_e}(h_e) = \prod_{e\in E(\gamma)} \sqrt{2j_e+1}\,[\pi(h_e)]_{j_e m_e n_e}\,, \tag{214}$$

where the $b_{j_e m_e n_e}(h_e)$ or $[\pi(h_e)]_{j_e m_e n_e}$ are the irreducible SU(2) representation of the holonomies along an edge e. Now we introduce a projector which projects the gauge variant SNFs to gauge invariant SNFs. For this purpose we split each edge $e \in E(\gamma)$ in γ into two segments s_1 and s_2 such that $e = s_1 \circ (s_2)^{-1}$, where s_1 is outgoing from the beginning point $b(e)$ of e and s_2 is outgoing from the final point $f(e)$ of e . As a consequence we get some additional vertices which are the intersection points of s_1 and s_2. We denote the new graph, consisting of the edges $\{s\}$, as γ'. The projector we need is then defined by

$$\mathcal{P} =: \int \mathrm{d}g \prod_{s\in E(\gamma');b(s)=v} b_{j_e m_e n_e}(g). \tag{215}$$

The idea behind the projector is that also the irreducible SU(2) representation transform under SU(2) gauge transformations like

$$b_{j_e}(h_e) \to b_{j_e}(h'_e) = b_{j_e}(g(b(e))h_e g(f(e))^{-1}) = b_{j_e}(g(b(e)))b_{j_e}(h_e)b_{j_e}(g(f(e))^{-1}), \tag{216}$$

where we suppressed the indices m_e, n_e to simplify the reading. So by application of the projector $\mathcal{P}$ to the SNF $T_{\gamma\vec{j}\vec{m}\vec{n}}(h)$ we access the beginning and final points of the edges which are the vertices of the graph and by integration over the group elements $g \in \mathrm{SU}(2)$ we integrate out the gauge variant parts. Since we used that we can identify our basis $|j_e, m_e\rangle$ with the angular momentum basis $|j, m\rangle$ used in quantum mechanics, we can also interpret this in terms of angular momentum coupling at the vertices. To begin with, we describe the coupling of two angular momenta j_1 and j_2 according to the theorem of ***Clebsch and Gordan***, see for example [118, 122].

Theorem [118, 122]: Clebsch & Gordan 2.4.2. *Given two irreducible representations π_{j_1}, π_{j_2} of* SU(2) *with angular momenta (weights) j_1 and j_2, their tensor product space splits into a direct sum of irreducible representations $\pi_{j_{12}}$ with angular momentum j_{12} taking values between $|j_1 - j_2| \leq j_{12} \leq j_1 + j_2$ such that*

$$\pi_{j_1} \otimes \pi_{j_2} = \pi_{j_1+j_2} \oplus \pi_{j_1+j_2-1} \oplus \ldots \oplus \pi_{|j_1-j_2+1|} \oplus \pi_{|j_1-j_2|}. \tag{217}$$

In terms of Hilbert spaces

$$\mathcal{H}^{(D)} = \mathcal{H}^{(D_1)} \otimes \mathcal{H}^{(D_2)} = \bigoplus_{j_{12}=|j_1-J_2|}^{j_1+j_2} \mathcal{H}^{(2j_{12}+1)} \tag{218}$$

with dimensions $D_1 = 2j_1 + 1$, $D_2 = 2j_2 + 1$ and $D = D_1 \cdot D_2$.

The angular momentum j_{12} is called the ***coupled angular momentum*** of j_1 and j_2. Now we have two optional basis for $\mathcal{H}^{(D)}$. First there is the tensor product basis $|j_1, m_1; j_2, m_2\rangle := |j_1, m_1\rangle \otimes |j_2, m_2\rangle$ and second the possibility to express $\mathcal{H}^{(D)}$ in terms of the ***coupled states*** $|j_1, j_2; J, M\rangle$, where $J := j_{12}(j_1, j_2)$ and $M := m_1 + m_2$. This on the contrary means that we can also expand one basis in terms of the other basis, i. e.

$$|j_1, j_2; J, M\rangle = \sum_M \langle j_1, m_1; j_2, m_2 | j_1, j_2; J, M\rangle \, |j_1, m_1; j_2, m_2\rangle. \tag{219}$$

The expansion coefficients $C_{m_1,m_2} := \langle j_1, m_1; j_2, m_2 | j_1, j_2; J, M\rangle \in \mathbb{R}$ are known as ***Clebsch-Gordon coefficients***. In the same manner as we coupled j_1 and j_2 to j_{12}, we can go on for N angular momenta, that is

$$\begin{aligned} & j_1, j_2 \to j_{12}, \\ & j_{12}, j_3 \to j_{123}, \\ & j_{123}, j_4 \to j_{1234}, \\ & \ldots \\ & j_{12\ldots(N-1)}, j_N \to J := j_{12\ldots N} \end{aligned} \tag{220}$$

which shows the recoupling scheme.

Usually, one couples the spins $\{j_e\}_{e\in E(\gamma)}$ to a total angular momentum J, such that a state of an angular momentum system expressed in the tensor product basis of the $|j_e, m_e\rangle$ can be expressed in a new basis $|J, M\rangle$, to simplify the notation the $\{j_e\}_{e\in E(\gamma)}$, respectively their partially coupled angular momenta, are left out. Mathematically, the coupling corresponds to a change of representation, where the map from one representation space to the other on is called an ***intertwiner*** I_v, realized by the collection of all Clebsch-Gordon coefficients at a vertex $v \in V(\gamma)$. Graphically expressed, the intertwiners sit a the vertices of a graph. The vectors $|J, M\rangle$ form the basis of their image space.

The Hilbert space at a vertex v for split edges has the form

$$\mathcal{H}_v = \left(\otimes_{s_1} j_{s_1^e}\right) \otimes \left(\otimes_{s_2} j_{s_2^e}\right), \tag{221}$$

where due to our split now all segments s of type one or two are outgoing from the vertex v. So to get a trivial tranformation behaviour at the vertices and therefore gauge invariance, the angular momenta or spins $j_{s_1^e}$ and $j_{s_2^e}$ need to couple to a total angular moment $J = 0$, and consequently $M = 0$ needs to be satisfied, then the resulting recoupling state $|0, 0\rangle$ is invariant under SU(2) gauge transformations. This makes also sense when one looks at the classical expression for the Gauß constraint in eq. (111) and notices that right and left invariant vector fields and their representations are associated with the beginning and final points of an edge, so their contributions should cancel in order to determine the gauge invariant Hilbert space $\mathcal{H}_{\text{kin}}$. Note that sometimes in the literature the term intertwiner is used only for the collection of all Clebsch-Gordon coefficients of the form $\langle 0,0|j_e,m_e\rangle$ at a vertex $v \in V(\gamma)$. Now the projector $\mathcal{P}$ can be expressed in terms of sums of scalar products of the form $\langle 0,0|j_e,m_e\rangle$ which are nothing else than Clebsch-Gordon coefficients. To complete the definition of the gauge invariant spin network states, one contracts the magnetic quantum numbers n_s which yields

$$T_{\gamma,\vec{j},\vec{I}} := \sum_{n_s} \left[\prod \langle 0,0|j_{s_1^e}, n_{s_1^e}; j_{s_2^e}, n_{s_2^e}\rangle\right] T_{\gamma',\vec{j},\vec{I},\vec{n}}, \tag{222}$$

where $T_{\gamma',\vec{j},\vec{I},\vec{n}}$ is the state after perfoming the momentum recoupling at each vertex $v \in V(\gamma)$. $\vec{I}$ is a vector which contains one entry for each vertex with one of all possible couplings to obtain the combined angular momentum of j_{s_1} and j_{s_2}. Finally, our auxillary construction of splitting an edge e into s_1 and s_2 is irrelevant, since their interior vertex is contracted with the same intertwiner. The $T_{\gamma,\vec{j},\vec{I}}$ form an orthonormal basis for $\mathcal{H}_{\text{kin}}$ because mapping from the tensor product basis to the recoupling basis (intertwiner) is a unitary transformation, see for example [118].

2.4.3 Diffeomorphism Constraint

The diffeomorphism constraint derived in section 1.3 modulo gauge transformations $G_j = 0$ is given by $C_a = -s\left({}^{(\beta)}F^j_{ab}\ {}^{(\beta)}E^b_j\right)$. For Lorentzian signature we set $s = -1$ and consider the smeared version

$$\vec{C}(\vec{N}) = \int_\sigma \mathrm{d}^3x\, N^a(x) \left({}^{(\beta)}F^j_{ab}\ {}^{(\beta)}E^b_j\right)(x), \tag{223}$$

where N^a is the shift vector. One can approximate $\vec{C}(\vec{N})$ in terms of holonomies and fluxes and realizes that the operator corresponding to infinitesimal diffeomorphisms does not exist on $\mathcal{H}_{\text{kin}}$ which is due to the fact that then the unitary operator $\exp(it\vec{C}(\vec{N}))$ would need to be strongly continous which is not the case. If $\exp(it\vec{C}(\vec{N}))$ is not strongly continuous, which is equivalent to weak continuity in case of unitary operators, then ***Stone's theorem*** 2.2.11 tells us that the operator for the generator $\vec{C}(\vec{N})$ does not exist, see also [9]. In the following we will show this explicitly. For this purpose let $\varphi_t^{\vec{C}(\vec{N})}$ be a one-parameter family of diffeomorphisms generated by the vector constraint $\vec{C}(\vec{N}) \neq 0$, then we have $\hat{U}(\varphi_t^{\vec{C}(\vec{N})}) = \exp(it\vec{C}(\vec{N}))$. Now choose a graph γ such that for all $t \in (0,\epsilon)$ for $\epsilon > 0$ we have $\varphi_t^{\vec{C}(\vec{N})}(\gamma) \neq \gamma$. Consider two identical SNFs $T_{\gamma,\vec{j},\vec{I}} = T_{\gamma',\vec{j}',\vec{I}'}$, since the SNF form an orthonormal basis we know that $\langle T_{\gamma,\vec{j},\vec{I}}, T_{\gamma,\vec{j},\vec{I}}\rangle = 1$. According to the definition of weak continuity 2.2.10, we consider

$$\lim_{t\to 0}\langle T_{\gamma,\vec{j},\vec{I}}, \hat{U}(\varphi_t)T_{\gamma,\vec{j},\vec{I}}\rangle = \lim_{t\to 0}\langle T_{\gamma,\vec{j},\vec{I}}, T_{\varphi_t^{\vec{C}(\vec{N})}(\gamma),\vec{j},\vec{I}}\rangle = 0 \neq 1 = \langle T_{\gamma,\vec{j},\vec{I}}, T_{\gamma,\vec{j},\vec{I}}\rangle, \tag{224}$$

which shows that indeed $\hat{U}(\varphi_t^{\vec{C}(\vec{N})})$ is not weakly continuous, so $\hat{\vec{C}}(\vec{N})$ does not exist.

However, this is not a problem, since finite spatial diffeomorphisms can be implemented unitarily due to the diffeomorphism covariance of the Ashtekar-Lewandowski representation, see

[95]. For all diffeomorphism $\varphi \in \mathrm{Diff}(\sigma)$ we can specify the action of the unitary operator $\hat{U}(\varphi)$, representing the finite diffeomorphisms, on a spin network function by

$$\hat{U}(\varphi)T_{\gamma,\vec{j},\vec{I}} = T_{\varphi(\gamma),\vec{j},\vec{I}}. \tag{225}$$

We remark that it is also possible to formulate the hypersurface deformation algebra in terms of finite instead of infinite diffeomorphisms and to implement this at the quantum level. As a consequence physical states ψ on $\mathcal{H}_{\mathrm{phys}}$ need to satisfy

$$\hat{U}(\varphi)\psi = \psi.$$

To determine the diffeomorphism invariant Hilbert space $\mathcal{H}_{\mathrm{diff}}$, we will apply the so-called ***refined algebraic quantization (RAQ) framework***, for details see [123, 124]. The first step of the RAQ consists in finding a sequence of spaces for a given Hilbert space $\mathcal{H}_{\mathrm{kin}}$, also called ***rigged Hilbert spaces*** or ***Gelfand' triple***

$$\mathcal{D}_{\mathrm{kin}} \subset \mathcal{H}_{\mathrm{kin}} \subset \mathcal{D}^*_{\mathrm{kin}}. \tag{226}$$

Here $\mathcal{D}_{\mathrm{kin}}$ is a dense subspace of the Hilbert space $\mathcal{H}_{\mathrm{kin}}$ whose elements in the case of LQG consist of the (gauge invariant) cylindrical functions, i.e. $\mathcal{D}_{\mathrm{kin}} = \mathrm{Cyl}$ and $\mathcal{D}^*_{\mathrm{kin}}$ is the so-called ***algebraic dual***. $\mathcal{D}^*_{\mathrm{kin}}$ consists of all linear functionals ℓ on $\mathcal{D}_{\mathrm{kin}}$, where all especially means that they do not need to be continuous. The algebraic dual $\mathcal{D}^*_{\mathrm{kin}}$ is per se equipped with the weak *-topology of pointwise convergence of nets (generalization of sequences), see [105].

In the second step we extend the action of the unitary operator of finite diffeomorphism $\hat{U}(\varphi)$ defined on $\mathcal{H}_{\mathrm{kin}}$ to linear functionals ℓ in $\mathcal{D}^*_{\mathrm{kin}}$ acting on $\mathcal{H}_{\mathrm{kin}}$ by

$$\left[\hat{U}_{\mathrm{ext}}(\varphi)\ell\right](f) = \ell(\hat{U}^\dagger(\varphi)f) = \ell(\hat{U}^{-1}(\varphi)f) \tag{227}$$

for all $f \in \mathcal{D}_{\mathrm{kin}}$, $\varphi \in \mathrm{Diff}(\sigma)$ and $\hat{U}_{\mathrm{ext}}(\varphi)$ on $\mathcal{D}^*_{\mathrm{kin}}$ is the operator extension of $\hat{U}(\varphi)$ on $\mathcal{H}_{\mathrm{kin}}$. Since the cylindrical functions are dense in $\mathcal{H}_{\mathrm{kin}}$ and the spin network functions lie dense in $\mathcal{D}_{\mathrm{kin}} = \mathrm{Cyl}$, we can concentrate our search for solutions to this domain. Let us define the multi-label $s := \{\gamma, \vec{j}, \vec{I}\}$, then $\varphi(s) := \{\varphi(\gamma), \vec{j}, \vec{I}\}$. For solutions to the diffeomorphism constraint, that is for invariant linear functionals, we demand that

$$\left[\hat{U}_{\mathrm{ext}}(\varphi)\ell\right](T_s) = \ell(\hat{U}^{-1}(\varphi)T_s) = \ell(T_{\varphi^{-1}(s)}) \stackrel{!}{=} \ell(T_s). \tag{228}$$

The solutions to these condition are linear functionals in the algebraic dual of the diffeomorphism invariant space $\mathcal{D}^*_{\mathrm{diff}} \subset \mathcal{D}^*_{\mathrm{kin}}$ and act on $\mathcal{H}_{\mathrm{kin}}$. Given that we have a linear functional $\ell \in \mathcal{H}_{\mathrm{kin}} \subset \mathcal{D}^*_{\mathrm{kin}}$, then the ***Riesz representation theorem*** [125] tells us that we can find an unique element $f_\ell \in \mathcal{H}_{\mathrm{kin}}$ such that ℓ can be expressed as $\ell = \langle f_\ell, . \rangle_{\mathrm{kin}}$ and $\langle ., . \rangle_{\mathrm{kin}}$ is the inner product on $\mathcal{H}_{\mathrm{kin}}$. We can concentrate on spin network functions T_s, since their finite linear combinations give rise to the cylindrical functions. All diffeomorphisms which relate a graph γ to its diffeomorphic image define an equivalence class $[s]$, more general equivalence classes generated by elements of a group are denoted as ***orbits***, given by

$$[s] := \{\varphi(s), \varphi \in \mathrm{Diff}(\sigma)\}. \tag{229}$$

Our motivation to work with the orbits is that we want to work with one representative s' of each equivalence class of diffeomorphisms. Taking all of the points mentioned above into account we reach at the solutions

$$\ell_{[s]}(T_{\tilde{s}}) = \sum_{s' \in [s]} \langle T_{s'}, T_{\tilde{s}} \rangle_{\text{kin}} \tag{230}$$

for any gauge invariant spin network function $T_{\tilde{s}}$. which indeed are invariant under the finite diffeomorphisms, that is $\hat{U}_{\text{ext}} \ell_{[s]}(T_{\tilde{s}}) = \ell_{[s]}(T_{\tilde{s}})$ as can easily be checked. This expression is always convergent, since the right hand side of eq. (230) will only contain finitely many non-vanishing terms due to the orthogonality of the spin network functions. In [102] it was shown that the Hilbert space $\mathcal{H}_{\text{kin}}$ decomposes into a direct sum of Hilbert spaces associated with each orbit $[s]$

$$\mathcal{H}_{\text{kin}} = \bigoplus_{[s]} \mathcal{H}^{[s]}_{\text{kin}}, \tag{231}$$

where each Hilbert space $\mathcal{H}^{[s]}_{\text{kin}}$ itself is composed as a direct sum $\mathcal{H}^{[s]}_{\text{kin}} = \bigoplus_{s' \in [s]} \mathcal{H}^{s'}_{\text{kin}}$.

Assume that we have managed to determine $\mathcal{D}^*_{\text{diff}}$, then we have the topological inclusion

$$\mathcal{D}_{\text{diff}} \subset \mathcal{H}_{\text{diff}} \subset \mathcal{D}^*_{\text{diff}}. \tag{232}$$

The map from $\mathcal{D}_{\text{kin}}$ to $\mathcal{D}^*_{\text{diff}}$ is the so-called ***rigging map*** $\eta(f)$, written as

$$\eta : \mathcal{D}_{\text{kin}} \to \mathcal{D}^*_{\text{diff}}, \quad f \mapsto \eta(f) \tag{233}$$

for all $f \in \mathcal{D}_{\text{kin}}$. It is useful to construct an inner product on the diffeomorphism invariant Hilbert space $\mathcal{H}_{\text{diff}}$, that is $\langle ., . \rangle_{\text{diff}}$. The rigging map $\eta(f)$ is basically given by a linear combination of the $\ell_{[s]}(.) = \sum_{s' \in [s]} \langle T_{s'}, . \rangle_{\text{kin}}$. Notice that, since $\mathcal{H}_{\text{kin}}$ splits into the $\mathcal{H}^{[s]}_{\text{kin}}$, the rigging map needs to be defined for each orbit $[s]$. Therefore, we choose a dense subspace $\mathcal{D}^{[s]}_{\text{kin}} \subset \mathcal{H}^{[s]}_{\text{kin}}$ and take its algebraical dual $\left(\mathcal{D}^{[s]}_{\text{kin}}\right)^*$. As an outcome the rigging map for each $[s]$ is defined by

$$\eta^{[s]}_a(T_{\tilde{s}}) := a_{[s]} \ell_{[s]}(T_{\tilde{s}}), \tag{234}$$

where $a_{[s]}$ is a non further specified real positive number. A general method to obtain the rigging map $\eta(f)$ is ***group averaging***, see definition 2.4.3 below. Notice that group averaging cannot be applied to the the diffeomorphism group $\text{Diff}(\sigma)$, since there exist uncountably infinitely many diffeomorphism which leave a given graph invariant. To obtain an explicit expression for the rigging map, we take those diffeomorphisms into account that leave our graph invariant based on our considerations to obtain a well defined element of $\left(\mathcal{D}^{[s]}_{\text{diff}}\right)^* \subset \left(\mathcal{D}^{[s]}_{\text{kin}}\right)^*$, see for example [9] for details on this. In the next section we will see that states which are solutions to the Hamiltonian constraint are also solutions to the diffeomorphism constraint.

2.4.4 Hamiltonian Constraint

For the derivation of the Hamiltonian constraint operator we follow the lines of [9, 126, 127]. To be able to work directly with the elements of a SU(2) Yang-Mills gauge theory, i.e. without the need to impose complicated reality conditions in the quantum theory, one chooses real connections A^j_a and densitized triads E^a_j. Besides from now on we set $\beta = 1$ and for Lorentzian signature we choose $s=-1$, then the Hamiltonian constraint, compare eq. (125), becomes

$$\begin{aligned}
C &= -\frac{1}{\sqrt{q}}\left({}^{(1)}F^j_{ab}\,\epsilon_{jk\ell}E^a_k E^b_\ell\right) - 2\sqrt{q}R \qquad (235)\\
&= -\frac{1}{\sqrt{q}}\left(F^j_{ab}\epsilon_{jk\ell}E^a_k E^b_\ell\right) - \frac{2}{\sqrt{q}}R_{ab}\delta^{k\ell}E^a_k E^b_\ell\\
&= \frac{i}{2\sqrt{q}}\mathrm{tr}(\sigma_j\sigma_k\sigma_\ell)\left(F^j_{ab}E^a_k E^b_\ell\right) - \frac{1}{\sqrt{q}}\mathrm{tr}(\sigma_k\sigma_\ell)\,R_{ab}E^a_k E^b_\ell\\
&= \frac{i}{2\sqrt{q}}\mathrm{tr}(\sigma_j\sigma_k\sigma_\ell)\,\frac{1}{2}\left(F^j_{ab}-F^j_{ba}\right)E^a_k E^b_\ell - \frac{1}{\sqrt{q}}\mathrm{tr}(\sigma_k\sigma_\ell)\,\frac{1}{2}\left(R_{ab}-R_{ba}\right)E^a_k E^b_\ell\\
&= \frac{1}{2\sqrt{q}}\mathrm{tr}\Big((-i\sigma_j)\frac{1}{2}\left(F^j_{ab}-F^j_{ba}\right)(-i\sigma_k)(-i\sigma_\ell)E^a_k E^b_\ell\Big)\\
&+ \frac{1}{\sqrt{q}}\mathrm{tr}\Big(\frac{1}{2}\left(R_{ab}-R_{ba}\right)(-i\sigma_k)(-i\sigma_\ell)E^a_k E^b_\ell\Big)\\
&= \frac{1}{2\sqrt{q}}\mathrm{tr}\Big(\frac{\tau_j}{2}\left(F^j_{ab}-F^j_{ba}\right)4\frac{\tau_k}{2}\frac{\tau_\ell}{2}E^a_k E^b_\ell\Big) + \frac{1}{\sqrt{q}}\mathrm{tr}\Big(\frac{1}{2}\left(R_{ab}-R_{ba}\right)4\frac{\tau_k}{2}\frac{\tau_\ell}{2}E^a_k E^b_\ell\Big)\\
&= \frac{2}{\sqrt{q}}\mathrm{tr}\big([F_{ab}+R_{ab}]\left[E^a,E^b\right]\big)\,.
\end{aligned}$$

In line three we used that for the Pauli matrices σ_j, $j=1,2,3$, we can reexpress $\delta^{k\ell}=\delta_{k\ell}=\frac{1}{2}\mathrm{tr}(\sigma_k\sigma_\ell)$ and $\epsilon_{jk\ell}=\frac{-i}{2}\mathrm{tr}(\sigma_j\sigma_k\sigma_\ell)$. Furthermore, we defined $\tau_j:=-i\sigma_j$ which are su(2) generators and we introduced the notation $F_{ab}:=F^j_{ab}\tau_j/2$ and $E^a:=E^a_j\tau_j/2$. Analogous we find for the Euclidean Hamiltonian constraint

$$C_{\mathrm{E}} = \frac{1}{\sqrt{q}}\left({}^{(1)}F^j_{ab}\,\epsilon_{jk\ell}E^a_k E^b_\ell\right) = -\frac{2}{\sqrt{q}}\mathrm{tr}\big(F_{ab}\left[E^a,E^b\right]\big)\,. \qquad (236)$$

It will prove to be useful not to write C in terms of F_{ab}, R_{ab} and E_a, but instead to use the expression for C_{E} in terms of K_{ab} and R_{ab}, namely

$$C_{\mathrm{E}} = -\sqrt{q}\left(K_{ab}K^{ab}-K^2\right) - \sqrt{q}R \qquad (237)$$

with this we can rewrite C, see eq. (125), as

$$\begin{aligned}
C &= -C_{\mathrm{E}} + 2C_{\mathrm{E}} + 2\sqrt{q}\left(K_{ab}K^{ab}-K^2\right) \qquad (238)\\
&= 2\sqrt{q}\left(K_{ab}K^{ab}-K^2\right) + C_{\mathrm{E}}\\
&= \frac{1}{\sqrt{q}}\left(K^\ell_a K^j_b - K^j_a K^\ell_b\right)E^a_j E^b_\ell + C_{\mathrm{E}}\\
&= \frac{4}{\sqrt{q}}\mathrm{tr}\big([K_a,K_b]\left[E^a,E^b\right]\big) + C_{\mathrm{E}}\\
&= (C-C_{\mathrm{E}}) + C_{\mathrm{E}},
\end{aligned}$$

where we set $K_a := K^j_a\tau_j/2$.

To include the $1/\kappa$ factor which appears in the Einstein Hilbert action one defines

$$H := \frac{1}{\kappa}C, \quad H^{\mathrm{E}} := \frac{1}{\kappa}C_{\mathrm{E}}. \qquad (239)$$

Notice that the classical Hamiltonian constraint is a real-valued function on the phase space of GR. It therefore suggests itself to search for an operator in the quantum theory which is self-adjoint or at least symmetric. However, from the point of view of the (semi)classical limit it is not necessary to construct a symmetric operator. Furthermore, the classical Hamiltonian constraint is not diffeomorphism invariant, but it is diffeomorphism covariant which will be carried over to the quantum level by the construction following below.

Here we follow the presentation of Thiemann given in [126, 127] to construct a non-symmetric Euclidean and Lorentzian Hamiltonian constraint operator. The construction of the symmetric version can also be found in [126, 127]. In the first step we replace the complicated curvature term R_{ab} by Poisson brackets using the subsequent quantities:

1. Volume of an open region R of σ

$$V(R) := \int_R \mathrm{d}^3x \sqrt{q} \tag{240}$$

2. Integrated densitized trace of the extrinsic curvature

$$\bar{K} := \int_\sigma \mathrm{d}^3x K_a^j E_j^a \tag{241}$$

There are two ***key identities*** which relate the volume V and the integrated densitized trace of the extrinsic curvature K to the terms appearing in the Hamiltonian constraint and between each other. Recall for $\beta = 1$ we have $K_a^j = A_a^j - \Gamma_a^j$ and $\Gamma_a^j = f[E]$ meaning that Γ_a^j is a homogeneous, rational function of E_j^a and its first derivatives are of order zero. The first key identity reads

$$\begin{aligned}\frac{\delta \bar{K}}{\delta E_j^a(x)} &= \frac{\delta}{\delta E_j^a(x)} \int_\sigma \mathrm{d}^3y\, K_b^k(y) E_k^b(y) = \frac{\delta}{\delta E_j^a(x)} \left[\int_\sigma \mathrm{d}^3y \, \left(A_b^k(y)E_k^b(y)\right) - \int_\sigma \mathrm{d}^3y \, \left(\Gamma_b^k(y)E_k^b(y)\right) \right] \\ &= A_a^j(x) - \Gamma_a^j(x) = K_a^j(x) = \frac{2}{\kappa}\{\bar{K}, A_a^j(x)\},\end{aligned} \tag{242}$$

where we used that $\{\bar{K}, \Gamma_a^j\} = \{\bar{K}, f(E)\} = 0$. The second key identity is

$$\left(\mathrm{sgn}(\det(e)) \frac{1}{\sqrt{q}} \epsilon_{jk\ell} E_k^a E_\ell^b \right)(x) = \epsilon^{abc} e_c^j(x) = 2\epsilon^{abc} \frac{\delta V(R)}{\delta E_j^c(x)} = \frac{4}{\kappa} \epsilon^{abc} \{V(R), A_c^j(x)\} \tag{243}$$

for any region R such that $x \in R$.

With the help of these key identities we find for any open neighbourhood R_x of $x \in \sigma$

$$\begin{aligned}\left(\mathrm{sgn}(\det(e))\,[H - H_{\mathrm{E}}]\right)(x) &= -\left(\frac{2}{\kappa}\right)^4 \epsilon^{abc} \mathrm{tr}\big(\{A_a(x), \bar{K}\}\{A_b(x), \bar{K}\}\{A_c(x), V(R_x)\}\big)\,, \\ \left(\mathrm{sgn}(\det(e))\, H_{\mathrm{E}}\right)(x) &= -\left(\frac{2}{\kappa}\right)^2 \epsilon^{abc} \mathrm{tr}(F_{ab}\{A_c(x), V(R_x)\})\,.\end{aligned} \tag{244}$$

We absorb the factor sgn(det(e)) into the lapse function N and write down the expressions for the smeared Hamiltonian and Euclidean Hamiltonian constraint, i.e. for $H(N) = \int_\sigma \mathrm{d}^3x\, N(x)H(x)$

and analogous for $H_{\mathrm{E}}(N)$, which then become

$$[H - H_{\mathrm{E}}](N) = -\left(\frac{2}{\kappa}\right)^4 \int\limits_\sigma \mathrm{d}^3x\, N(x)\epsilon^{abc}\mathrm{tr}\big(\{A_a(x),\bar{K}\}\{A_b(x),\bar{K}\}\{A_c(x),V(R)\}\big)\,, \tag{245}$$
$$H_{\mathrm{E}}(N) = -\left(\frac{2}{\kappa}\right)^2 \int\limits_\sigma \mathrm{d}^3x\, N(x)\epsilon^{abc}\mathrm{tr}(F_{ab}\{A_c(x),V(R)\})\,.$$

Since the holonomy-flux algebra gives rise to the Hilbert space $\mathcal{H}_0$ we also want to recast the connections A_a and their curvature F_{ab} in terms of holonomies in order to be able to find a representation of the Hamiltonian constraint on $\mathcal{H}_0$ or $\mathcal{H}_{\mathrm{kin}}$ in case that we solve the Gauß constraint first. For this purpose we fill out σ by tetrahedra which intersect each other only in lower dimensional submanifolds (surfaces) and whose volume depends on a small parameter ϵ. We call this a ***triangulation*** $T(\epsilon)$ of σ. The triangulation will be defined such that for ϵ getting smaller the number of tetrahedra is increasing to make sure that σ is always filled out with tetrahedra. The triangulation should be adapted to an underlying graph in order to give reasonable meaning to the limit $\epsilon \to 0$. In the following we want to explain what it means to ***adapt the triangulation to an underlying graph*** γ***.*** Let $\triangle := \triangle_\epsilon \in T(\epsilon)$ be an analytic tetrahedron, where we will suppress the ϵ dependence of the tetrahedra in the following. Denote the edges of the tetrahedron by $e_I(\triangle)$, $I = 1,2,3$ and their intersection point by $v(\triangle)$. We assume that all vertices are at least three-valent. In case of two-valent vertices one can make them three-valent by adding an additional edge not intersecting γ in any other point except the vertex v which means that its tangent is transversal to all other tangents of edges of γ at v. The final Euclidean Hamiltonian constraint operator $\hat{H}^{\mathrm{E}}(N)$ annihilates functions based on graphs with two-valent vertices. Without loss of generality we choose the edges to have an outgoing orientation from $v(\triangle)$. Otherwise, one can subdivide the edges like in the case of the derivation of the volume operator in section 2.3. Moreover, we introduce the notions of ***segments*** s_I and ***arcs*** a_{IJ}. A segment s_I of e_I is a part of e_I such that it starts at v with outgoing orientation and does not include any other endpoint v_I of e_I apart from v. An arc a_{IJ} intersects two edges e_I and e_J in their endpoints and we define a ***loop*** $\alpha_{IJ}(\triangle) := e_I(\triangle) \circ a_{IJ}(\triangle) \circ e_J^{-1}(\triangle)$ that has positive orientation with respect to the boundary $(I,J) = (1,2),(2,3),(3,1)$.

In order to cast eq.(245) in terms of holonomies we choose two embedded edges $e(t) : [0,1] \to \sigma$ and $e'(t') : [0,1] \to \sigma$ with $t \to e(t)$, $t' \to e'(t')$ such that the have a common starting point $v = e(0) = e'(0)$ and we set $e_\epsilon(t) := e(\epsilon t)$, analogous for $e'(t')$, for $0 < \epsilon < 1$ and $t,t' \in [0,1]$. Here we abuse the notation and use the same symbols for the edges and their embeddings. The expansion of the holonomy $h_\epsilon(A_a^j)$ in powers of ϵ reads

$$h_{e_\epsilon}(A_a^j) = \mathbb{1}_2 + \epsilon\dot{e}(0)A_a^j(v)\frac{\tau_j}{2} + \mathcal{O}(\epsilon^2), \tag{246}$$

where dot denotes the derivative of $e(t)$ with respect to the parameter t.

To rewrite the term containing the curvature F_{ab}, we need to introduce a suitable loop. For our embedding of the edges $e(t) : [0,1] \to \sigma$ and likewise $e(t')$ this loop in a coordinate neighbourhood is given by

$$\alpha_{e_\epsilon,e'_\epsilon}(t) = \begin{cases} e_\epsilon(4t) & 0 \le t \le 1/4 \\ e_\epsilon(1) + e'_\epsilon(4t-1) - v & 1/4 \le t \le 1/2 \\ e'_\epsilon(1) + e_\epsilon(3-4t) - v & 1/2 \le t \le 3/4 \\ e'_\epsilon(4-4t) & 3/4 \le t \le 1. \end{cases} \tag{247}$$

Then the expansion of the corresponding holonomy in powers of ϵ yields

$$h_{\alpha_{e_\epsilon,e'_\epsilon}} = \mathbb{1}_2 + \epsilon^2 F^j_{ab}\dot{e}^a(0)\dot{e}'^b(0)\frac{\tau_j}{2} + \mathcal{O}(\epsilon^3). \tag{248}$$

The integral over σ can roughly be decomposed into a sum over tetrahedra which we will explain in more detail for the derivation of the quantized expression. Then eq. (245) becomes

$$\begin{aligned}\left(H - H^{\mathrm{E}}\right)(N) &= \frac{1}{3}\left(\frac{2}{\kappa}\right)^4 \sum_{\triangle\in T(\epsilon)} N_v \epsilon^{IJK}\mathrm{tr}\Big(h_{e_I(\triangle)}\{h^{-1}_{e_I(\triangle)},\bar{K}\}h_{e_J(\triangle)}\{h^{-1}_{e_J(\triangle)},\bar{K}\} \\ &\qquad h_{e_K(\triangle)}\{h^{-1}_{e_K(\triangle)},V\big(R_{v(\triangle)}\big)\}\Big) + \mathcal{O}(\epsilon^2) \\ H^{\mathrm{E}}(N) &= \frac{1}{3}\left(\frac{2}{\kappa}\right)^2 \sum_{\triangle\in T(\epsilon)} N_v \epsilon^{IJK}\mathrm{tr}\Big(h_{\alpha_{IJ}(\triangle)}h_{e_K(\triangle)}\{h^{-1}_{e_K(\triangle)},V\big(R_{v(\triangle)}\big)\}\Big) + \mathcal{O}(\epsilon^2),\end{aligned} \tag{249}$$

where we have defined $N_v := N(v(\triangle))$. For any triangulation the expressions in eq. (249) converge pointwise on M to the expressions in eq. (245). The constant terms vanish under the action of the Poisson bracket. Actually, to replace the integral over σ by the sum over tetrahedra is a very rough description of the situation, since there is still some "space" around the vertex left with is not filled by the tetrahedra. To obtain the correct prefactor in the quantum description we need to treat the integral over sigma in the subsequent sense. We will not go into details of the construction of the so-called ***mirror tetrahedra*** here which can be found in [126], but it is not hard to imagine that at each vertex we actually have eight tetrahedra constructed from a triple of edges e_I, e_J, e_K and their prolongations or "mirror edges". The eight tetrahedra, constructed from these edges, saturate the region around a vertex v. Let $D(\triangle)$ be the closed region in σ filled by the eight tetrahedra constructed from a triple e_I, e_J, e_K. Their union is $D(v) = \bigcup_{v(\triangle)=v} D(\triangle)$ and their complement with respect to $D(v)$ is $\bar{D}(\triangle) := D(v) - D(\triangle)$. The left space $\bar{D} := \sigma - \bigcup_{v\in V(\gamma)} D(v)$ is triangulated arbitrarily, but will not give any contribution. Thus, the integral according to [126] can be rewritten as

$$\begin{aligned}\int_\sigma &= \int_{\sigma-\bigcup_{v\in V(\gamma)} D(v)} + \sum_{v\in V(\gamma)}\int_{D(v)} = \int_{\bar{D}} + \sum_{v\in V(\gamma)}\frac{1}{E(v)}\sum_{v(\triangle)=v}\left[\int_{D(\triangle)} + \int_{\bar{D}(\triangle)}\right] \\ &= \sum_{\triangle'\in\bar{D}}\int_{\triangle'} + \sum_{v\in V(\gamma)}\frac{1}{E(v)}\sum_{v(\triangle)=v}\left[\sum_{\triangle'\in D(\triangle)}\int_{\triangle'} + \sum_{\triangle'\in\bar{D}(\triangle)}\int_{\triangle'}\right].\end{aligned} \tag{250}$$

Due to the symmetry of the problem we can make the replacement

$$\sum_{\triangle'\in D(\triangle)}\int_{\triangle'} \to 8\int_{\triangle}. \tag{251}$$

as in the limit $\epsilon \to 0$ all the tetrahedra shrink to their base point which is a vertex of the graph. The remaining sums over integrals containing tetrahedra in $\bar{D}$ and $\bar{D}(\triangle)$ vanish. Now we have re-expressed H^{E} and H in terms of quantities we know how to quantize. One more subtlety we need to take into account is that classically it does not matter whether we quantize H^{E} and H or their complex conjugates $\bar{H}^{\mathrm{E}}$ and $\bar{H}$ because they are real-valued, however for the construction of the solutions to the constraints, we need the adjoint operators. Observe that $\hat{H}$ does not need to be self-adjoint, see [126, 127], so there might be a difference between $\hat{H}$ and $\hat{H}^\dagger$ on the quantum level. For $\bar{H}^{\mathrm{E}}$ and $\bar{H}$ the corresponding operators acting on a function cylindrical with respect to a graph γ are given by

$$\left[\left(\hat{H}-\hat{H}^{\mathrm{E}}\right)(N)\right]^\dagger f_\gamma = \frac{128}{3\kappa\left(i\ell_P^2\right)^2}\sum_{v\in V(\gamma)}\frac{N(v)}{E(v)}\sum_{v(\triangle)=v}\epsilon^{IJK} \tag{252}$$
$$\times\,\mathrm{tr}\Big(h_{e_I(\triangle)}\left[h^{-1}_{e_I(\triangle)},\hat{\bar{K}}\right]h_{e_J(\triangle)}\left[h^{-1}_{e_J(\triangle)},\hat{\bar{K}}\right]h_{e_K(\triangle)}\left[h^{-1}_{e_K(\triangle)},\hat{V}\big(R_{v(\triangle)}\big)\right]\Big)f_\gamma,$$
$$\left[\hat{H}^{\mathrm{E}}(N)\right]^\dagger f_\gamma = \frac{32}{3\kappa i\ell_P^2}\sum_{v\in V(\gamma)}\frac{N(v)}{E(v)}\sum_{v(\triangle)=v}\epsilon^{IJK}\mathrm{tr}\Big(h_{\alpha_{IJ}(\triangle)}h_{e_K(\triangle)}\left[h^{-1}_{e_K(\triangle)},\hat{V}\big(R_{v(\triangle)}\big)\right]\Big)f_\gamma$$

with $\hat{\bar{K}} := \frac{i}{\hbar}\left[\hat{H}^{\mathrm{E}}(1),\hat{V}(\sigma)\right]$ which comes from the classical identity for the integrated densitized trace of the extrinsic curvature $\bar{K} = -\{H^{\mathrm{E}}(1),V(\sigma)\}$ for a constant lapse function $N=1$. Application of $\hat{H}^{\mathrm{E}}(N)$, respectively $\left[\hat{H}^{\mathrm{E}}(N)\right]^\dagger$, to a cylindrical function results again in a cylindrical function which depends on additional edges. The algebra of two Hamiltonian constraint operators can be shown to be non-anomalous, i.e. the algebra is closed. More on the action of the Lorentzian Hamiltonian operator and especially the calculation of its matrix elements can be found in [128].

The ***solutions to the Hamiltonian constraint operator*** have to be states on the diffeomorphism invariant Hilbert space $\psi\in\mathcal{H}_{\mathrm{diff}}\subset\mathcal{D}^*_{\mathrm{diff}}$ which should satisfy

$$\left((\hat{H}(N))^\dagger\psi\right)f := \psi\left(\hat{H}(N)f\right) = 0 \tag{253}$$

for arbitrary smooth lapse functions $N\in C^\infty(\sigma)$ and cylindrical functions $f\in\mathcal{D}$ in the (dense) domain of $\hat{H}(N)$. If we would impose the condition $(\hat{H}(N))^\dagger\psi=0$, we cannot require ψ to be diffeomorphism invariant, since according to the hypersurface deformation algebra the Hamiltonian constraint does not leave $\mathcal{H}_{\mathrm{diff}}$ invariant. Meaning that we needed to solve the Hamiltonian before the diffeomorphism constraint. To construct the solutions to the non-symmetric Euclidean and Lorentzian Hamiltonian constraint we will introduce a couple of definitions. The construction of the solutions to the symmetric version of the Hamiltonian constraint is even more complicated and we will not display it here, for their construction see [127].

Following [127], we begin with the definition of an ***extraordinary vertex***. An extraordinary vertex is a tri-valent vertex which is the intersection of two analytic curves $c, c'\subset\gamma$, that is $v = c\cap c'$, such that v is an endpoint of c but not of c'. An ***extraordinary edge*** is an edge whose endpoints are extraordinary vertices v_1, v_2. There is an at least tri-valent vertex v of γ which is such that at least three edges incident at it have linearly independent tangents at v and there are two edges $s_1, s_2\subset\gamma$ which connect v and v_1, v_2 and which have linearly independent tangents at v. We call v the typical vertex associated with e. Further, to construct the solution of the Hamiltonian constraint we need rules to choose suitable spin-network functions, therefore we present the definition of a ***spin net***.

Definition [127]: Spin-Net 2.4.1.

1. *A spin-net is a pair $\omega=(\gamma,\vec{j})$ consisting of a graph $\gamma\in\Gamma$ and a colouring of the edges of γ with spins $j>0$ such that the set of intertwiners (vertex contractors) $\vec{I}$ compatible with the data $\gamma,\vec{j}$ is not empty. We will denote the set of all spin-nets by W.*

2. *The subset $W_0 \subset W$ is defined to be the set of all $(\gamma, \vec{j}) \in W$, where γ is a piecewise analytic graph, all of whose extraordinary edges carry a spin $j > 1/2$. We also set $\overline{W}_0 = W - W_0$.*

3. *Given $\omega = (\gamma, \vec{j}) \in W$ there exists a unique spin-net $\omega_0(\omega) = (\gamma_0(\gamma), \vec{j}_0(\vec{j})$, called the **source of** ω and which is defined by the subsequent algorithm:*
First let $\tilde{\gamma}$ be a copy of γ which we dye in white. If $\omega \notin W_0$ remove all the extraordinary edges e of γ which carry spin $1/2$ in γ to obtain a graph γ'. Now if s_1, s_2 are the segments of γ which connect the extraordinary edge e with its typical vertex then dye s_1, s_2 black in $\tilde{\gamma}$ to produce $\tilde{\gamma}'$. Iterate the procedure with $\gamma', \tilde{\gamma}'$ instead of $\gamma, \tilde{\gamma}$. The procedure must come to an end after a finite number of steps because γ had only a finite number of edges. The final γ' is the searched for $\gamma_0(\gamma)$ which by construction is unique. Its colouring $\vec{j}_0$ is obtained as follows: Each edge e of $\gamma_0(\gamma)$ has finite segments s which is dyed in white in the final $\tilde{\gamma}$ and which belongs to an edge e' of γ. We define $\vec{j}_0(\vec{j})$ by requiring that the colour of e is the same as that of e': It is clear that the pair $(\gamma_0, \vec{j}_0)$ defines an element of W_0: it is an element of W because the space of vertex contractors associated with a tri-valent vertex as that given by the endpoints of an extraordinary edge is one-dimensional and that it lies in W_0 follows from the construction.

The idea behind this abstract construction is to assume that we have a final graph on which we applied the Hamiltonian constraint. A rough analogy is to think about this like applying a creation operator several times on an initial state unless a certain final state is reached. Then the upcoming definition enables us to go "backwards" to the initial state or "forwards" to a derived state.

Definition [127]: Derived Spin-Nets 2.4.2.

1. *Let $\omega_0 = (\gamma_0, \vec{j}_0) \in W_0$. We define inductively finite sets of spin-nets $\omega = (\gamma, \vec{j}) \in \bar{W}_0$ with source ω_0 as follows:*

   (a) *Let $W^{(0)}(\omega_0) := \{\omega_0\}$.*

   (b) *Given $W^{(n)}(\omega_0)$ take any $\omega = (\gamma, \vec{j}) \in W^{(n)}(\omega_0)$ and construct elements of $\omega' = (\gamma', \vec{j}')$ of $W^{(n+1)}(\omega_0)$ as follows: add precisely one more extraordinary edge e to γ in all possible, topologically inequivalent ways. Furthermore, if v is the typical vertex for e and if $e_i = s_i \circ s_i'$, $i = 1, 2$, $s_i, s_i' = \varnothing$ carries spin j_i, where s_1, s_2 connect v to the endpoints of e then we define up to four colourings for $\gamma \cup e$ as follows:*

      i. *The extraordinary edge e is coloured with spin $1/2$.*
      ii. *s_i' is coloured with spin j_i as before.*
      iii. *s_i is coloured with spin $j_i' := j_i \pm 1/2$.*
      iv. *The edges of $\gamma - \{e_1, e_2\}$ carry the same spin as in γ.*
      v. *From the colourings of $\gamma \cup e$ so obtained we keep only those which admit a non-empty set of vertex contractors.*
      vi. *Define $\gamma' = \gamma \cup e$, $(\gamma - s_1) \cup e$, $(\gamma - s_2) \cup e$, $(\gamma - s_1 - s_2) \cup e$ if (j_1', j_2') is $(\neq 0, \neq 0)$, $(0, \neq 0)$, $(\neq 0, 0)$, $(0, 0)$ respectively. The set of data $\omega' = (\gamma', \vec{j}')$ (at most four) $\omega = (\gamma, \vec{j})$ and for each e extraordinary for γ so obtained comprises the set $W^{(n+1)}(\omega_0)$. The finite set $W^{(n)}(\omega_0)$ will be called the set of **derived spin-nets** of level n with source ω_0.*

2. *We will denote the associated set of equivalence classes of spin-nets under diffeomorphisms by $\left[W^{(n)}(\omega_0)\right]$ which itself, of course, depends only on the equivalence class $[\omega_0]$ of ω_0.*

Finally, to be able to define states which satisfy the diffeomorphism constraint as well as the Hamiltonian constraint we need to perform a ***group averaging***.

Definition [127]: Group Average 2.4.3.

1. *Let $T_{\gamma,\vec{j},\vec{I}}$ be a spin-network state. Its group average is defined by the following well-defined distribution on $\Phi = Cyl^{\infty}(\overline{\mathcal{A}/\mathcal{G}})$ which is also a solution to the diffeomorphism constraint, i. e. a subset of $\mathcal{H}_{\text{diff}}$,*
$$T_{[\gamma],\vec{j},\vec{I}} := \sum_{\gamma' \in [\gamma]} T_{\gamma',\vec{j},\vec{I}} \tag{254}$$
where $[\gamma]$ denoted the orbit of γ under smooth diffeomorphisms of σ which preserves analycity of γ.

2. *The **group average** $[f]$ **of any cylindrical function** f is defined by first decomposing it into spin-network states and then averaging each of the spin-network states separately.*

According to the following theorem the solutions to the (Lorentzian) Hamiltonian constraint $\hat{H}$ and dffeomorphism constarint are then given by:

Theorem 1.1 [127]: Group Average 2.4.4. *Each distributional solution to all constraints of Lorentzian quatum gravity is a finite linear combination of states Ψ of the following two types:*
Type I)
$\psi = [f]$ where f is an arbitrary linear combination of spin-network states based on spin-nets $\omega_0 \in W_0$.
Type II)
$\psi = [f]$ where f is a certain linear combination of spin-network which are constructed from spin-nets in $\overline{W}_0$.

The solutions of type I are trivial in the sense discussed in the proof of Theorem 1.1 in [127]. Therefore, we only try to explain the solutions of type II in more detail as also done in the proof of Theorem 1.1 in [127].

Let $f = \sum_T a^{(n)}_{[T]}([\omega_0])T$. The sum extends over

1. All spin-nets $\omega \in W^{(n)}(\omega_0)$ for some $\omega_0 = (\gamma_0, \vec{j}_0)$ and some $n > 0$.
2. All spin-network states T compatible with precisely on of these ω. We denote the set of all spin-network states T compatible with precisely on of these ω by $\mathcal{S}^{(n)}(\omega_0)$.

Let $[s] = [\gamma], \vec{j}, \vec{I}$ be a label for the diffeomorphism invariant and gauge invariant with respect to the Gauß constraint SNF $T_{[s]}$, compare section 2.4.3, and define $\left[\mathcal{S}^{(n)}(\omega_0)\right] := \{[s]_{s\in\mathcal{S}^{(n)}(\omega_0)}\}$. Then the ***solution for the non-symmetric Hamiltonian constraint operator*** is of the form

$$\psi := \sum_{k=1}^{N} \sum_{[s]\in\left[\mathcal{S}^{(n_k)}(\omega_0)\right]} a^{(n_k)}_{[s]}([\omega_0])T_{[s]}. \tag{255}$$

The tricky part are the constants $a^{(n_k)}_{[s]}([\omega_0])$ which need to be determined from eq. (253). So in principle for the non-symmetric Hamiltonian constraint operator we are able to determine the complete kernel which then gives us the physical Hilbert space. We see that the physical Hilbert space is actually the one already constructed in [102]. This is closely related to the point that it is diffeomorphism covariantly like its classical counter part. The Hamiltonian constraint operator acts by annihilating, creating, and re-routing the spins (angular) momenta in a spin-network. In the case for the symmetric operator one has to do even more work and there is no complete solution, but solutions can be calculated case by case as explained in [127].

Co-Authorship Declaration for Part III

Contribution of Almut Vetter to the publication: "Comparison Between Dirac and Reduced Quantization in LQG-Models with Klein-Gordon Scalar Fields" published in Acta Phys. Polon. Supp., 2017, doi:10.5506/APhysPolBSupp.10.339

As a co-author I confirm that Almut Vetter contributed significantly to the results of the publication "Comparison Between Dirac and Reduced Quantization in LQG-Models with Klein-Gordon Scalar Fields". This involves her work on the conceptual questions, the technical methods as well as the content of this article. In particular this involves all computations necessary to obtain the final results presented in the publication as well as how these results compare to the classical results underlying the Dirac quantization approach. The presentation of the work in the thesis summarizes well her contributions to the publication.

Kristina Giesel

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Contribution of Almut Vetter to the publication: "Reduced loop quantization with four Klein–Gordon scalar fields as reference matter" published in Class. Quant. Grav., 2019, doi:10.1088/1361-6382/ab26f4

As a co-author I confirm that Almut Vetter contributed significantly to the results of the publication "Reduced loop quantization with four Klein–Gordon scalar fields as reference matter". This involves her work on the conceptual questions, the technical methods as well as the content of this article. In particular this involves all computations necessary to obtain the final results presented in the publication as well as developing ideas and strategies how a reduced phase space quantization can be implemented for the model under consideration and how this compares to the Dirac quantization approach. The presentation of the work in the thesis summarizes well her contributions to the publication.

Kristina Giesel

Kristina Giesel

Part III
Construction of Physical Hamiltonian Operators

Most of the content in this part has been published in [129] and [130]. Sections of text within this part have been reused from an article published in Classical and Quantum Gravity [130]. IOP Publishing Ltd is not responsible for any errors or omissions in the text included within this thesis. The Version of Record of the published article is available online at the URL stated in [130]. However, this thesis contains additional calculational and theoretical work.

3 Reduced Phase Space Quantization

Instead of Dirac quantization as applied in section 2 we can also perform a so-called ***reduced phase space quantization***. In this case we solve the constraints, which is meant by "reduce", at the classical level and then we try to find a representation of the resulting observable algebra. Usually, it is more difficult to find a representation of the observable algebra than of the kinematical algebra. However, in case we add a suitable reference matter action to the Einstein Hilbert action we are able to rewrite the constraints linearly in the momenta of the reference fields. After we have rewritten the constraints, we can use them to apply the so-called ***observable map***, see section 5. The observable map maps the kinematical quantities and their algebra to observables and the observable algebra. Whether the reference matter action was suitable is reflected in how the resulting algebra of the rewritten constraints looks like. In the ideal case the observable algebra is isomorphic to the hypersurface deformation algebra which means that we will be able to use the standard LQG kinematical Hilbert space representation. We do not need to solve all constraints at the classical or at the quantum level. It is also possible to solve some of the constraints at the classical level and then solve the remaining constraints via Dirac quantization at the quantum level. In the upcoming calculations we add four (modified) Klein-Gordon scalar fields to the Einstein-Hilbert action. Afterwars we rewrite the Hamiltonian and spatial diffeomorphism constraint. In the following we solve these constraints at the classical level but we will use Dirac quantization to solve the remaining Gauss constraint at the quantum level. We denote the reference matter fields, often called "clocks", by φ^I and their conjugate momenta by π_I, where I denotes an element of an index set with countable cardinality $\mathcal{I}$ and each index usually marks a field. Mathematically, the procedure can be described as follows: By adding a matter action to the Einstein-Hilbert action we extend the phase space. Now given a phase space with canonical coordinates (x, p_x) one can, at least locally, subdivide the phase space into two canonically conjugate subsets $(\varphi^I, \pi_I)_{I\in\mathcal{I}}$ that corresponds to our reference matter and $(q^a, p_a)_{a\in\mathcal{A}}$, where $\mathcal{A}$ is an index set with countable cardinality, that corresponds to our gravitational (ADM or Ashtekar) variables. Then one can solve the first class constraints C_I for the momenta π_I which results in equivalent constraints $\tilde{C}_I(\varphi^I, \pi_I, q^a, p_a) = \pi_I + h_I(\varphi^I, q^a, p_a)$ for functions $h_I(\varphi^I, q^a, p_a)$ depending on the remaining coordinates. In case that the function h_I only depends on the (q^a, p_a), and not on the reference matter φ^I, i.e $h_I = h_I(q^a, p_a)$ one says that the system ***deparametrizes***. The next step is to set $\tilde{C}_I(\varphi^I, \pi_I, q^a, p_a) = 0$ and to solve for $h_I(\varphi^I, q^a, p_a) = \pi_I$. We will see that h_I gives rise to a so-called ***physical Hamiltonian*** $\mathbf{H}_{\text{phys}}$ that generates the evolution of the observables. In the subsequent sections we explain the concepts of constraints and observables in section 4 as well as the observable map in section 5 in detail. We shortly classify the reference matter models in section 6. Afterwards we apply the knowledge from sections 4 to 6 to the case of four (modified) Klein-Gordon scalar fields and display our results in sections 7, 8 and 9 before we conclude in section 10.

4 Constraints and Observables

Observables are usually understood to be measurable quantities. Therefore, they play a central role in physics because they are accessible by experiment and can be used to falsify or support a physical theory. From their understanding as measurable quantities in quantum theory one draws the conclusion that operators should be self-adjoint, since then they have real eigenvalues. In gauge theories, i.e. theories that are invariant under certain transformations we demand the measurable quantities, that is the observables, to be invariant under the transformation in consideration. This can on the algebraical level be expressed by the requirement that observables commute with the generators of the corresponding gauge transformations which are first class constraints. In the following we summarize some definitions, where we stick to the presentations given in [17, 18]. Let $\mathcal{I}$ be an arbitrary index set with countable cardinality. Moreover, let $\{C_I\}_{I\in\mathcal{I}}$ be a system of ***first class constraints***, that is a system of functions $C_I = C_I(g)$ on a phase space Γ, where g denotes a point in the phase space Γ, which satisfy

$$\{C_I, C_J\} = \sum_K f_{IJ}^K C_K \tag{256}$$

for all indices I, J and phase space functions $f_{IJ}^K = f_{IJ}^K(g)$, $g \in \Gamma$. If the f_{IJ}^K are constants, they will be called ***structure constants*** otherwise they will be called ***structure functions***. A function $O = O(g)$, $g \in \Gamma$, on the phase space Γ is then called a ***weak Dirac observable*** if and only if there exist non-vanishing functions $g_I^J = g_I^J(g)$, $g \in \Gamma$, on the phase space for all I such that

$$\{C_I, O\} = \sum_J g_I^J C_J. \tag{257}$$

This means that the Poisson bracket $\{C_I, O\}$ is going to vanish on the ***constraint hypersurface***, that is the submanifold of the classical phase space selected by $C_I = 0$ for all I. One says that $\{C_I, O\}$ is ***weakly vanishing*** on the constraint hypersurface denoted by

$$\{C_I, O\} \approx 0 \tag{258}$$

for all I. More general one says that a ***relation holds weakly*** and denotes it by $\approx$ in case that equality is only valid on the constraint hypersurface. For $g_I^J = 0$ the equality holds exactly and O is called a ***strong Dirac observable***.

Given a set of first class constraints $\{C_I\}_{I\in\mathcal{I}}$ and chosen a corresponding set of reference matter $\{\varphi^I\}_{I\in\mathcal{I}}$, we want them to be, at least weakly, canonically conjugate, that is

$$\{\varphi^I, C_J\} \approx \delta_J^I. \tag{259}$$

This requirement is important for the construction of the observables we are going to introduce in the next section. However, in general the reference matter φ^I and first class constraints C_I form a ***second class system***, which means that

$$\{\varphi^I, C_J\} =: A_J^I \tag{260}$$

with A^I_J being an invertible matrix. Now we can define the equivalent set of constraints

$$C'_I := \sum_J (A^{-1})^J_I C_J. \tag{261}$$

With this new set of constraints $\{C'_I\}_{I\in\mathcal{I}}$, as one can easily show, we have indeed

$$\{\varphi^I, C'_J\} \approx \delta^I_J, \quad \{C'_I, C'_J\} \approx 0 \tag{262}$$

for all indices I, J. This procedure is called ***weak Ablization*** and is discussed in [17, 19].

Now we come to the ***relational formalism*** based on an observation made and investigated by Rovelli, see for example [21, 22]. Rovelli observed that there are basically two different kinds of observables in physics which he calls ***partial and complete observables***. In [22] the following definitions where given:

Definition [22]: Partial Observable 4.1. *A partial observable is a physical quantity to which we can associate a (measuring) procedure leading to a number.*

Definition [22]: Complete Observable 4.1. *A complete observable is a physical quantity whose classical value or in quantum theory whose probability distribution can be predicted by the theory.*

Roughly, "relational formalism" in this context means: a function $F(T)$ takes a certain value $F(T_I)$ when a clock or more general reference variable T takes a certain value T_I and if the function $F(T)$ is the outcome of a physical theory, it will be a complete observable. In case that the values for F and T are measurable separately each of them is a partial observable. These concepts together with the framework of the Hamiltonian flow generated by first class constraints C_I, which is explained in section 5, were used in [17, 19] to construct observables for constrained systems described by a Hamiltonian.

5 Observable Map

Large parts of this section have been published in [130]. Now we want to describe the construction of the observables for a given set of first class constraints $\{C_I\}_{I\in\mathcal{I}}$ and a chosen set of reference matter "clocks" $\{\varphi^I\}_{I\in\mathcal{I}}$ which are at least weakly canonically conjugate, that is $\{\varphi^I, C_J\} \approx \delta^I_J$. If this is not the case, we can define a new set of constraints $\{C'_I\}_{I\in\mathcal{I}}$, as explained in section 4, which satisfies this property. Consider the ***Hamiltonian vector field*** X_I associated with C_I defined by $X_I := \{C_I, .\}$. In the following constructions we make successive use of the fact that the X_I mutually weakly commute. For each constraint C_I we introduce an arbitrary real number β^I and consider the sum of Hamiltonian vector fields

$$X_\beta := \sum_I \beta^I X_I. \tag{263}$$

Let f be a smooth function on the phase space, then the ***Hamiltonian flow*** $f \to \alpha_\beta(f)$ on the set of smooth functions on the phase space is given by

$$\alpha_\beta(f) := \exp(X_\beta)\cdot f = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} X^n_\beta \cdot f \ , \tag{264}$$

here the multiple action of the Hamiltonian vector field on f is given by $X^n_\beta \cdot f := \{C_\beta, f\}_{(n)}$, where $C_\beta := \sum_I \beta^I C_I$ and $\{.,.\}_{(n)}$ denotes the iterated Poisson bracket defined by $\{C_\beta, f\}_{(0)} = f$ and $\{C_\beta, f\}_{(n)} = \{C_\beta, \{C_\beta, f\}_{(n-1)}\}$. The Hamiltonian flow generated by the C_I represents the gauge transformations on the phase space. The additional factor $(-1)^n$ in α_β comes from the fact that we use the Poisson bracket convention $\{q^A, p_B\} = \delta^A_B$ here, in contrast to [9, 26] and part II where $\{q^A, p_B\} = -\delta^A_B$ is used. As an alternative to inserting (-1), we could define $X^n_\beta \cdot f := \{f, C_\beta\}_{(n)}$ with $\{f, C_\beta\}_{(0)} = f$ and $\{f, C_\beta\}_{(n)} = \{\{f, C_\beta\}_{(n-1)}, C_\beta\}$.

By making use of the Jacobi identity for the Poisson bracket as well as the definitions of the Hamiltonian vector fields and the Hamiltonian flow, one can show that the Hamiltonian flow defines a ***canonical transformation (symplectomorphism)*** and an ***algebra isomorphism (Poisson automorphism)*** on the algebra of functions on the phase space, see for instance [17, 18], that is

$$\alpha_\beta(f + f') = \alpha_\beta(f) + \alpha_\beta(f'), \quad \alpha_\beta(f f') = \alpha_\beta(f)\alpha_\beta(f'), \quad \{\alpha_\beta(f), \alpha_\beta(f')\} = \alpha_\beta(\{f, f'\}). \tag{265}$$

In accordance with the relational formalism we construct with the help of the Hamiltonian flow a map that returns the value of f at those values where the reference matter φ^I as a function on the phase space takes the values τ^I. Therefore, we choose another set of real numbers $\{\tau^I\}_{I\in\mathcal{I}}$ and look for those values of the gauge parameters β^I for which $\alpha_\beta(\varphi^I) = \tau^I$. The application of α_β to the reference matter gives $\alpha_\beta(\varphi^I) \approx \varphi^I + \beta^I$, which can easily be solved for β^I yielding $\beta^I = \tau^I - \varphi^I$. We will denote this equation for short as $\beta = \tau - \varphi$ suppressing the indices. This input is enough to obtain a map for the phase space function f which gives us an observable related to f. We refer to this map as the ***observable map***

$$O_f(\tau) := [\alpha_\beta(f)]_{\beta=\tau-\varphi}\,. \tag{266}$$

During the calculation of the observable map it is important first to calculate the Poisson brackets or the action of the vector fields X_β on the phase space functions f respectively, since then the β^I are considered as constants and afterwards to set $\beta = \tau - \varphi$ because by that the β^I become phase space dependent. In [17, 18, 19] it was proven that $O_f(\tau)$ weakly commutes with the constraints C_I for all $I \in \mathcal{I}$, i.e.

$$\{O_f(\tau), C_I\} \approx 0, \tag{267}$$

hence $O_f(\tau)$ is indeed a weak Dirac observable. From the properties of the Hamiltonian flow in eq. (265) follow the addition and pointwise multiplication of the observable map

$$O_f(\tau) + O_g(\tau) = O_{f+g}(\tau), \quad O_f(\tau)O_g(\tau) \approx O_{fg}(\tau). \tag{268}$$

Therefore, the multi-parameter family of maps $O^\tau : f \to O_f(\tau)$ is a homomorphism from the algebra of functions on phase space to the algebra of weak Dirac observables as explicitly shown in [17, 18, 19, 20]. However, concerning the Poisson bracket we do not any longer have a Poisson automorphism by the multi-parameter family of maps $O^\tau : f \to O_f(\tau)$. Despite that it is possible to find a Poisson homomorphism by the introduction of the ***Dirac bracket***. For any two smooth phase space functions the Dirac bracket is defined as

$$\{f, g\}^* := \{f, g\} - \sum_{I,J} \{f, C_I\}(A^{-1})^I_J \{\varphi^J, g\} + \sum_{I,J} \{g, C_I\}(A^{-1})^I_J \{\varphi^J, f\}. \tag{269}$$

with invertible matrix $A^I_J := \{\varphi^I, C_J\}$. Usually, we try to find "clocks" such that the matrix A^I_J is weakly equal to δ^I_J on the constraint surface, that is $\approx \delta^I_J$ or use Abelization as explained in section 4. On the constraint hypersurface we then have the weak equalities

$$\{O_f(\tau), O_g(\tau)\} \approx \{O_f(\tau), O_g(\tau)\}^* \approx O_{\{f,g\}^*}(\tau), \tag{270}$$

which shows that the multi-parameter family of maps $O^\tau : f \to O_f(\tau)$ is a Poisson homomorphism, also explicitly proven in [18, 20].

Assume that we have a smooth phase space function $f = f(q^a, p_a)$ that only depends on the canonically conjugate coordinates (q^a, p_a) but not on the elementary variables of the reference matter (φ^I, π_I). In this setting we can by making use of the Taylor expansion and the addition and pointwise multiplication in eq. (268) show that

$$O_f(\tau) = f(O_{q_A}, O_{p^A})(\tau), \tag{271}$$

i.e. the observable $O_f(\tau)$ corresponding to the function f is the same as the function f of the observables corresponding to q^a and p_a.

Remember that with the help of the reference fields and their conjugate momenta we can derive equivalent constraints

$$\tilde{C}_I(\varphi^I, \pi_I, q^a, p_a) = \pi_I + h_I(\varphi^I, q^a, p_a) \tag{272}$$

to the constraints C_I. Let us discuss the construction of the observables for the elementary variables (q^a, p_a) with respect to the new constraints $\tilde{C}_I$. Since q^a and p_a both commute with all momenta π_I, we can consider the Hamiltonian vector field associated with the h_I's instead of defining X_β via the equivalent constraints $\tilde{C}_I$. Moreover, for the reason that also q^a and p_a commute with all reference fields φ^I, we can already when applying X_β to f, for a function f that only depends on (q^a, p_a), replace β by $\tau - \varphi$ which yields to the following form of the observable map

$$O_f(\tau) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} X_\tau^n \cdot f, \tag{273}$$

where X_τ is the Hamiltonian vector field of the function

$$H_\tau = \sum_I (\tau^I - \varphi^I) H_I \tag{274}$$

and $H_I := O_{h_I}(\tau)$ denotes the observable associated with each h_I. We denote the observables associated with q^a and p_a by $Q^a(\tau) := O_{q^a}(\tau)$ and $P_a(\tau) := O_{p_a}(\tau)$.

Another point is that if we restrict to functions that do only depend on q^a and p_a, the Dirac bracket will according to eq. (269) reduce to the Poisson bracket because those f commute with all reference matter φ^I. In particular for the algebra of the observables $Q^a(\tau)$ and $P_a(\tau)$ we obtain

$$\{Q^a(\tau), P_b(\tau)\} = \{O_{q^a}(\tau), O_{p_b}(\tau)\} = O_{\{q^a, p_b\}}(\tau) = O_{\delta^a_b}(\tau) = \delta^a_b, \tag{275}$$

showing that the reduced phase space has a very simple symplectic structure in terms of the coordinates Q^a, P_a, an important property if the quantization of such systems is considered.

Let us add a few more observations: the observable associated with the reference matter φ^I is given by

$$O_{\varphi^I}(\tau) = \left[\alpha_\beta(\varphi^I)\right]_{\beta=\tau-\varphi} = \tau^I \tag{276}$$

and therefore is just a constant function on the phase space. According to eq. (272) the momenta π_I can be expressed as functions of the observables $O_{\varphi^I}(\tau) = \tau^I$, $Q^a(\tau)$ and $P_a(\tau)$ because on the constraint surface we have

$$\Pi_I = O_{\pi_I}(\tau) = -O_{h_I}(\tau) = -h_I(\tau^I, Q^a(\tau), P_a(\tau)) = -H_I. \tag{277}$$

The system deparametrizes in case that we have $h_I(q^a, p_a)$, that is h_I in eq. (272) depends on (q^a, p_a) only but not on the reference matter φ^I. If none of the h_I depends on the reference fields φ^I, we will get $\{\varphi^I, \tilde{C}_J\} = \delta^I_J$ and $\{h_I, h_J\} = 0$. From the last Poisson bracket follows that, if all constraints $\tilde{C}_I$ are linearly in the momenta π_I, then the associated constraint algebra will be Abelian $\{\tilde{C}_I, \tilde{C}_J\} = 0$. Consequently, we have $\{h_I, \tilde{C}_J\} = 0$ which shows that each h_I is already a Dirac observable, i.e. $H_I := O_{h_I}(\tau) = h_I$. Moreover, from the Abelian constraint algebra we can conclude that also the associated Hamiltonian vector fields commute not only on the constraint surface but on the entire phase space. Meaning that all weak equalities that we have used above can be replaced by strong equalities here. Since $h_I = h_I(q^a, p_a)$ is a function of q^a and p_a only, once the observables for the elementary variables $Q^a(\tau)$ and $P_a(\tau)$ are constructed, we obtain H_I as $H_I = O_{h_I}(\tau) = h_I(Q^a, P_a)(\tau)$ by the map given in eq. (271).

Finally, we consider again an observable $O_f(\tau)$ associated with a function that depends on q^a and p_a only. We want to formulate the evolution of such observables. Certainly, the evolution cannot be generated by the constraints because by construction $O_f(\tau)$ Poisson commutes with all constraints. However, $O_f(\tau)$ gives us the value of f when the reference matter φ^I as functions on phase space take the values τ^I. Let us without loss of generality denote the reference matter associated with physical time by φ^0 and the values that it takes by τ^0. Then the time evolution of $O_f(\tau)$ can be described by the derivative of $O_f(\tau)$ with respect to τ^0, since this encodes how $O_f(\tau)$ changes with time τ^0. Considering the form of $O_f(\tau)$ in eq. (273), we can explicitly compute this derivative and as shown in [18] for a deparametrized system one obtains

$$\frac{\partial O_f(\tau)}{\partial \tau^0} = \{O_f(\tau), H_0\}, \tag{278}$$

where $H_0 := \int d^3x\, O_{h_0}$ is the integrated observable associated with h_0 that occurs in the constraint $\tilde{C}_0 := \pi_0 + h_0(q^a, p_a)$ associated with reference matter φ^0 that we interpret as reference matter for the temporal coordinate. In the following we will call H_0 the ***physical Hamiltonian***, later denoted as $\mathbf{H}_{\text{phys}}$ because in contrast to the constraint $\tilde{C}_0$, which is generating gauge transformations, H_0 does not vanish on the constraint surface and therefore can be understood as a true Hamiltonian which generates evolution with respect to physical time τ^0. Since h_0 does not depend on φ^0 and on any other reference matter, the final physical Hamiltonian H_0 is time independent.

Above we mainly discussed the case where the system deparametrizes but as has been shown in [23] and will be also important for the models discussed in the following, if the system does not deparametrize, the function h_0 *will depend on the partial derivatives of* φ^0 *only.* In this case the final physical Hamiltonian H_0 will be still independent of time.

For simplicity we only considered functions on a phase space here. Despite that we also can and will apply the techniques discussed here to field models taking care of the mathematical details regarding field theories.

6 Classification of Reference Matter Models

Large parts of this section have been published in [130]. As discussed in [23] reference matter models can be classified as ***type I and type II models***. Type I models can be characterized by containing two pairs of four scalar fields and usually form a second class system. If one reduces the system with respect to the second class constraints one pair of the four scalar fields can be expressed in terms of the remaining degrees of freedom and one ends up with a first class system for which the remaining four scalar fields can be used as reference matter. This first class system is then the starting point for the reduced phase space quantization. Thus, a full reduction with respect to the Hamiltonian and spatial diffeomorphism constraint is possible. An example for such a model is the Brown-Kuchař dust model, that has been introduced by Kuchař et al in their seminal papers [25, 131, 132] and has been used in [5] to perform a reduced phase space quantization of Loop Quantum Gravity.

In contrast, type II models only partially reduce the phase space with respect to the constraints, since these models only include one reference field usually used as reference matter associated with the Hamiltonian constraint. An example for a type II model that has been applied in the context of Loop Quantum Gravity is the model in [1], where one Klein-Gordon scalar field has been considered as reference matter.

7 Four Klein-Gordon Scalar Fields as Reference Matter

Large parts of this section have been published in [129] and [130]. In this section we consider the model of the gravitational field coupled to four Klein-Gordon scalar reference fields and derive the physical Hamiltonian of this model. This model can be understood as the natural type I model associated with the one scalar field model in [1] which originally was considered because it is the full Loop Quantum Gravity generalization of the Ashtekar-Pawlowski-Singh (APS) model introduced in [24]. We denote the four Klein-Gordon scalar fields by φ^I with labels $I, J = 0, \cdots, 3$. The action of the total system under consideration is given by

$$S[g,\varphi^I] = \int\limits_M d^4Y\sqrt{g}R^{(4)} - \frac{1}{2}\int\limits_M d^4Y\sqrt{g}\,\delta_{IJ}\,g^{\mu\nu}\varphi^I_{,\mu}\varphi^J_{,\nu} = S^{\mathrm{geo}} + S^{\varphi}, \qquad (279)$$

where $g_{\mu\nu}$ is the space-time metric, $g := |\det(g_{\mu\nu})|$, $R^{(4)}$ denotes the four-dimensional Ricci scalar and $\mu, \nu = 0, \cdots, 3$ are space-time indices. Note that the indices $I, J = 0, \cdots, 3$ are just internal ones labeling the reference matter fields. They have no relation to the space-time indices. We choose our signature convention for the space-time metric tensor $g_{\mu\nu}$ to be $(-,+,+,+)$. The comma denotes a partial derivative with respect to the space-time metric $g_{\mu\nu}$ or later on with respect to the spatial metric q_{ab}. Next we want to perform the ADM split.Let (M, g) be some globally hyperbolic four dimensional manifold diffeomorphic to $\mathbb{R} \times \chi$, where χ is a three dimensional manifold, as discussed in section 1.2. The χ_t denote the spacelike leaves of a foliation which correspond to the images of a one parameter family of embeddings $t \mapsto Y_t$, where $Y(t,x) \equiv Y_t(x)$. The timelike normals to the leaves are given by $n^\mu = \frac{1}{n}[Y^\mu_{,t} - n^a Y^\mu_{,a}]$. They are future oriented which requires $n > 0$. The three metric q on χ is then obtained from the pull-back of the space-time or four metric $g_{\mu\nu}$ under the embeddings $q_{ab}(t,x) = Y^\mu_{,a}Y^\nu_{,b}g_{\mu\nu}$. We perform the ADM split using $\sqrt{|\det(g)|} = n\sqrt{\det(q)} =: n\sqrt{q}$, $g^{\mu\nu} = n^\mu n^\nu + q^{ab}Y^\mu_{,a}Y^\nu_{,b}$ and define $\varphi^J_n := n^\mu \varphi^J_{,\mu}$, $\varphi^J_{,a} := Y^\mu_{,a}\varphi^J_{,\mu}$ then our action for the Klein-Gordon fields becomes

$$S^\varphi = +\frac{1}{2}\sum_{J=0}^{3}\int\limits_{\mathbb{R}}\mathrm{d}t\int\limits_{\chi}\mathrm{d}^3x\, n\,\sqrt{q}\left(\left[\varphi^J_n\right]^2 - q^{ab}\varphi^J_{,a}\varphi^J_{,b}\right) \tag{280}$$

with $a, b = 1, 2, 3$.

7.1 Total Action in Canonical Form

Next we determine the canonically conjugate momenta and constraints of the total action $S = S^{\mathrm{geo}} + S^\varphi$. S^{geo} is the ordinary Einstein-Hilbert action in the ADM frame, see for example part II section 1.1 and [26]. The canonically conjugate momenta corresponding to the Klein-Gordon fields are

$$\begin{aligned}\pi_J := \frac{\delta S}{\delta\dot\varphi^J} &= \sum_{J=0}^{3}\int\limits_{\mathbb{R}}\mathrm{d}t\int\limits_{\chi}\mathrm{d}^3x\, n\,\sqrt{q}\varphi^I_n\frac{\delta\varphi^I_n}{\delta\dot\varphi^J} \\ &= \sum_{J=0}^{3}\int\limits_{\mathbb{R}}\mathrm{d}t\int\limits_{\chi}\mathrm{d}^3x\, n\,\sqrt{q}\varphi^I_n\frac{1}{n}\delta^I_J\delta^{(4)}(x,y) \\ &= \sqrt{q}\varphi^I_n\delta^I_J = \sqrt{q}\varphi^J_n,\end{aligned} \tag{281}$$

where dot denotes the derivative with respect to the time parameter t in the ADM frame. The canonically conjugate momenta corresponding to the lapse n and to the components of the shift vector n^a are

$$\begin{aligned}p := z := \frac{\delta S}{\delta\dot n} &= 0, \\ p_a := z_a := \frac{\delta S}{\delta\dot n_a} &= 0.\end{aligned} \tag{282}$$

They cannot be solved for the corresponding velocities which means that they are primary constraints.

Now the total action in canonical form after performing the Legendre transformation looks like

$$\begin{aligned}S = &\int\limits_{\mathbb{R}}\mathrm{d}t\int\limits_{\chi}\mathrm{d}^3x\left(p\dot n + p_a\dot n^a + \frac{1}{\kappa}p^{ab}\dot q_{ab} + \sum_{J=0}^{3}\pi_J\dot\varphi^J\right) \\ &-\int\limits_{\mathbb{R}}\mathrm{d}t\int\limits_{\chi}\mathrm{d}^3x\, h_{\mathrm{primary}}\end{aligned} \tag{283}$$

and h_{primary} is given by

$$h_{\mathrm{primary}} = \frac{1}{\kappa}p^{ab}\dot q_{ab} - \mathcal{L}_{\mathrm{geo}} + \sum_{J=0}^{3}\pi_J\dot\varphi^J - \mathcal{L}_\varphi + \nu z + \nu_a z^a. \tag{284}$$

The term $\frac{1}{\kappa}p^{ab}\dot q_{ab} - \mathcal{L}_{\mathrm{geo}}$ gives rise to the geometric part of the Hamiltonian and diffeomorphism constraints c^{geo} and c^{geo}_a, for example they can be found in [9, 26] and compare part II section

1.3. They are given by

$$\begin{aligned}\kappa c^{\mathrm{geo}} &= \frac{1}{\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right) p^{ab}p^{cd} - \sqrt{q}R^{(3)}, \\ \kappa c_a^{\mathrm{geo}} &= -2q_{ac}\, D_b p^{bc}.\end{aligned} \tag{285}$$

From $\sum_{J=0}^{3} \pi_J \dot{\varphi}^J - \mathcal{L}_\varphi$ we determine the part of the constraints which belongs to the four Klein-Gordon scalar fields. Writing out the terms in detail leads to

$$\begin{aligned}&\sum_{J=0}^{3} \pi_J \dot{\varphi}^J - \mathcal{L}_\varphi \\ &= \sum_{J=0}^{3} \pi_J \dot{\varphi}^J - \frac{1}{2}\sum_{J=0}^{3} n\sqrt{q}\left(\left[\varphi_n^J\right]^2 - q^{ab}\varphi^J_{,a}\varphi^J_{,b}\right) \\ &= n\,\frac{1}{2}\sum_{J=0}^{3}\left[\frac{{\pi_J}^2}{\sqrt{q}} + \sqrt{q}q^{ab}\varphi^J_{,a}\varphi^J_{,b}\right] + n^a \sum_{J=0}^{3}\pi_J\varphi^J_{,a} \\ &=: n\, c^\varphi + n^a\, c_a^\varphi,\end{aligned} \tag{286}$$

where we used that $\pi_J = \sqrt{q}\varphi_n^J$ and we solved $\varphi_n^J = \frac{1}{n}(\dot{\varphi}^J - n^a\varphi^J_{,a})$ for the velocities, that is

$$\dot{\varphi}^J = n\varphi_n^J + n^a\varphi^J_{,a} = n\frac{\pi_J}{\sqrt{q}} + n^a\varphi^J_{,a}. \tag{287}$$

By defining $c^{\mathrm{tot}} := c^{\mathrm{geo}} + c^\varphi$ and $c_a^{\mathrm{tot}} := c_a^{\mathrm{geo}} + c_a^\varphi$ we can write the primary Hamiltonian as

$$\begin{aligned}H_{\mathrm{primary}} &= \int_\chi \mathrm{d}^3x\, h_{\mathrm{primary}} \\ &= \int_\chi \mathrm{d}^3x\, \left(nc^{\mathrm{tot}} + n^a c_a^{\mathrm{tot}} + \nu z + \nu^a z_a\right).\end{aligned} \tag{288}$$

In summary we end up with the following expression for the canonical action

$$\begin{aligned}&S[q_{ab}, p^{ab}, n, p, n^a, p_a, \varphi^J, \pi_J] \\ &= \int_{\mathbb{R}} dt \int_\chi d^3x \left(\dot{q}_{ab}p^{ab} + \dot{\varphi}^J\pi_J + \dot{n}p + \dot{n}^a p_a - \left[nc^{\mathrm{tot}} + n^a c_a^{\mathrm{tot}} + \nu z + \nu^a z_a\right]\right),\end{aligned} \tag{289}$$

with

$$z := p, \quad z_a := p_a, \quad c^{\mathrm{tot}} := c^{\mathrm{geo}} + c^\varphi, \quad c_a^{\mathrm{tot}} := c_a^{\mathrm{geo}} + c_a^\varphi \tag{290}$$

and

$$\begin{aligned}\kappa c^{\mathrm{geo}} &= \frac{1}{\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right)p^{ab}p^{cd} - \sqrt{q}R^{(3)}, \\ c^\varphi &= \frac{\delta^{IJ}\pi_I\pi_J}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}\delta_{IJ}q^{ab}\varphi^I_{,a}\varphi^J_{,b}, \\ \kappa c_a^{\mathrm{geo}} &= -2q_{ac}D_b p^{bc}, \\ c_a^\varphi &= \pi_J\varphi^J_{,a},\end{aligned} \tag{291}$$

here $\kappa = 16\pi G$ where G is Newton's gravitational constant, D_a is the torsion free metric compatible connection with respect to the ADM metric as defined in section 1.2, $q := \det(q_{ab})$ and z, z_a are primary constraints of the canonical action.

7.2 Constraint Stability Analysis

To analyze the time evolution of the primary constraints z and z_a under the primary Hamiltonian we notice that the non-vanishing Poisson brackets on the phase space are given by

$$\begin{aligned} \{q_{cd}(x), p^{ab}(y)\} &= \kappa \delta^a_{(c}\delta^b_{d)}\delta^{(3)}(x,y), \\ \{n(x), p(y)\} &= \delta^{(3)}(x,y), \\ \{n^b(x), p_a(y)\} &= \delta^a_b \delta^{(3)}(x,y), \\ \{\varphi^I(x), \pi_J(y)\} &= \delta^I_J \delta^{(3)}(x,y), \end{aligned} \tag{292}$$

where we use a different Poisson bracket convention here than we did in part II to make our work easier to compare to other results in the literature, see for example [1, 26, 133]. The analysis of the stability of the primary constraints shows that c^{tot} and c^{tot}_a are the secondary constraints of the system.

$$\begin{aligned} \dot{z} &= \{z, H_{\text{primary}}\} = \{p, H_{\text{primary}}\} = -c^{\text{tot}}, \\ \dot{z}_a &= \{z_a, H_{\text{primary}}\} = \{p_a, H_{\text{primary}}\} = -c^{\text{tot}}_a. \end{aligned} \tag{293}$$

No tertiary constraints arise, since we are in a similar situation as in [26], for a prove see appendix A there. As expected each of the four reference fields φ^I contributes to the Hamiltonian and diffeomorphism constraint with the standard expression of a Klein-Gordon scalar field. The set of constraints $\{z, z_a, c^{\text{tot}}, c^{\text{tot}}_a\}$ is first class. We go over to the reduced ADM phase space for which $z \approx 0$ and $z_a \approx 0$ and in this phase space we can treat lapse n and shift n^a as Langrange multipliers.

7.3 Step 1: Construction of Observables

Now we will use the formalism introduced in section 5 and apply it to the four Klein-Gordon scalar fields model in order to construct observables with respect to the Hamiltonian and spatial diffeomorphism constraint. For this purpose as a first step we have to rewrite the Hamiltonian as well as the spatial diffeomorphism constraint in an equivalent form as described in sections 3 and 5 such that the set of resulting constraints becomes weakly Abelian, compare section 4. To achieve this we will use the same strategy as in [26], that is first we solve the four constraints for the four reference field momenta π_J and then we apply the so-called Brown-Kuchař mechanism in order to ensure that the final physical Hamiltonian is given in deparametrized form.

7.3.1 Weakly Abelian Set of Constraints

We start with the spatial diffeomorphism constraint c^{tot}_a and want to solve it for π_j. In order that the scalar fields φ^j with $j = 1, 2, 3$ serve as good reference fields we have to assume that $\varphi : \chi \to \mathcal{S}$ is a diffeomorphism, where $\mathcal{S}$ denotes the scalar field manifold consisting of the values the fields φ^j can take. We denote by φ^a_j the inverse of $\varphi^j_{,a}$, such that $\varphi^a_j \varphi^j_{,b} = \delta^a_b$, $\varphi^a_k \varphi^j_{,a} = \delta^j_k$. Using this we can solve for π_j and get

$$c^{\text{tot}}_a = 0 \quad \Leftrightarrow \quad \pi_j = -\varphi^b_j \left(c^{\text{geo}}_b + \pi_0 \varphi^0_{,b}\right) =: -\widetilde{h}_j(q_{ab}, p^{ab}, \varphi^0, \varphi^j, \pi_0) =: -\widetilde{h}_j. \tag{294}$$

Further, we want to solve c^{tot} for π_0. Considering the explicit form of c^{tot} in eq. (291) we make use of the constraint condition $c^{\text{tot}} = c^{\text{geo}} + c^{\varphi} = 0$ multiply with $2\sqrt{q}$ and reinsert the result for the momenta π_j from eq. (294) into it, where the last step is known as the ***Brown-Kuchař***

mechanism. Note that we apply the Brown-Kuchař mechanism not in its standard form here because then we would replace $q^{ab}\varphi^0_{,a}\varphi^0_{,b}$ by $\frac{q^{ab}(c^{\rm geo}_a+\pi_j\varphi^j_{,a})(c^{\rm geo}_b+\pi_j\varphi^j_{,b})}{\pi_0^2}$ but here we use the spatial diffeomorphism constraint to replace π_j. The advantage of this is that we get at most a quadratic equation in π_0 and not a fourth order one as in [1] which in general yields to a more complicated form of the final physical Hamiltonian. These steps lead to

$$-2\sqrt{q}c^{\rm geo} = {\pi_0}^2 + \delta^{jk}\varphi^a_j\left(c^{\rm geo}_a + \pi_0\varphi^0_{,a}\right)\varphi^b_k\left(c^{\rm geo}_b + \pi_0\varphi^0_{,b}\right) + q\delta_{JK}q^{ab}\varphi^J_{,a}\varphi^K_{,b}. \tag{295}$$

In an intermediate step we calculated the term

$$\begin{aligned}
&\delta^{jk}\varphi^a_j\left(c^{\rm geo}_a + \pi_0\varphi^0_{,a}\right)\varphi^b_k\left(c^{\rm geo}_b + \pi_0\varphi^0_{,b}\right)\\
&= \delta^{jk}\varphi^a_j\varphi^b_k\left[c^{\rm geo}_a c^{\rm geo}_b + \pi_0 c^{\rm geo}_a\varphi^0_{,b} + \pi_0 c^{\rm geo}_b\varphi^0_{,a} + \varphi^0_{,a}\varphi^0_{,b}{\pi_0}^2\right]\\
&= \delta^{jk}\varphi^a_j\varphi^b_k c^{\rm geo}_a c^{\rm geo}_b + \delta^{jk}\varphi^a_j\varphi^b_k\left(c^{\rm geo}_a\varphi^0_{,b} + c^{\rm geo}_b\varphi^0_{,a}\right)\pi_0 + \delta^{jk}\varphi^a_j\varphi^b_k\varphi^0_{,a}\varphi^0_{,b}{\pi_0}^2.
\end{aligned}$$

This is a quadratic equation for the scalar field momentum π_0 and can be rewritten as

$$\begin{aligned}
0 = &\left(1 + \delta^{jk}\varphi^a_j\varphi^b_k\varphi^0_{,a}\varphi^0_{,b}\right){\pi_0}^2 + \delta^{jk}\varphi^a_j\varphi^b_k\left(c^{\rm geo}_a\varphi^0_{,b} + c^{\rm geo}_b\varphi^0_{,a}\right)\pi_0\\
&+ q\delta_{JK}q^{ab}\varphi^J_{,a}\varphi^K_{,b} + \delta^{jk}\varphi^a_j\varphi^b_k c^{\rm geo}_a c^{\rm geo}_b + 2\sqrt{q}c^{\rm geo}.
\end{aligned} \tag{296}$$

Let us define the following abbreviations

$$\begin{aligned}
a &:= \left(1 + \delta^{jk}\varphi^a_j\varphi^b_k\varphi^0_{,a}\varphi^0_{,b}\right),\\
b &:= \delta^{jk}\varphi^a_j\varphi^b_k\left(c^{\rm geo}_a\varphi^0_{,b} + c^{\rm geo}_b\varphi^0_{,a}\right),\\
c &:= q\delta_{JK}q^{ab}\varphi^J_{,a}\varphi^K_{,b} + \delta^{jk}\varphi^a_j\varphi^b_k c^{\rm geo}_a c^{\rm geo}_b + 2\sqrt{q}c^{\rm geo},
\end{aligned} \tag{297}$$

then solving for π_0 yields

$$\pi_0 = -\frac{b}{2a} \pm \sqrt{\left(\frac{b}{2a}\right)^2 - \frac{c}{a}} =: -h(q_{ab}, p^{ab}, \varphi^0, \varphi^j) =: -h. \tag{298}$$

Note that the application of the Brown-Kuchař mechanism in its standard way does not result in a form of the Hamiltonian constraint that can be written linearly in π_0 and a function that does not depend on the remaining scalar field momenta π_j. In order to ensure later on that the physical Hamiltonian density is positive we choose the plus sign for the square root in the definition of h. Now we will use the results in eq. (294) and eq. (298) to write down an equivalent set of constraints that is linearly in the scalar field momenta. Here we leave out the tilde in the new constraints to simplify the notation. We obtain

$$\begin{aligned}
c^{\rm tot} &:= \pi_0 + h(q_{ab}, p^{ab}, \varphi^0, \varphi^j),\\
c^{\rm tot}_j &:= \pi_j + h_j(q_{ab}, p^{ab}, \varphi^0, \varphi^j),
\end{aligned} \tag{299}$$

where we used $\pi_0 = -h$ to obtain from $\widetilde{h}_j$ a function h_j that no longer depends on the momentum π_0. The result here also coincides with [132], where a model with eight scalar fields was considered to implement the harmonic gauge condition. There the second class model can be reduced to a first class model with four remaining scalar fields of the Klein-Gordon type. We realize that neither the new Hamiltonian constraint nor the spatial diffeomorphism constraint is in deparametrized form for the reason that the function h as well as the functions h_j still depend on the scalar fields φ^J, $J = 0, \dots, 3$. However, as pointed out in [23] in case these functions depend only on spatial derivatives of the reference fields the final resulting physical Hamiltonian will still be time-independent and this is exactly the case for the present model as we will show in the next subsection. In contrast to the old constraints the constraints shown in eq. (299) are weakly Abelian and can thus be used to construct observables for the geometric degrees of freedom using the four scalar fields as reference fields. In the following we will construct the observables in two steps. First we reduce with respect to the spatial diffeomorphism constraint and afterwards with respect to the Hamiltonian constraint.

7.3.2 Explicit Construction of the Observables

For the construction of the observables we closely follow [26], where four dust reference fields are used. Likewise to the case of the dust reference fields, we will construct the final observable in two steps. First, we derive spatially diffeomorphism invariant quantities. For this purpose, as in [26], we define the smeared constraint

$$K_{\beta_1} := \int\limits_{\chi} d^3x\, \beta_1^j c_j^{\mathrm{tot}}. \tag{300}$$

Observables with respect to K_{β_1} are given by

$$O^{(1)}_{f,\{\varphi^j\}}(\sigma) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \Big[\{K_{\beta_1}, f\}_{(n)}\Big]_{\beta_1^j = \sigma^j - \varphi^j}. \tag{301}$$

For the dust reference fields in [26] an explicit form of the iterated Poisson bracket $\{K_{\beta_1}, f\}_{(n)}$ in terms of vector fields v_j acting on a scalar g by $v_j \cdot g(x) := S^a_j g_{,a}$ was derived, where S^j denotes the reference dust fields and S^a_j the inverse of $S^j_{,a}$. All the steps used [26] in order to prove the explicit form of the iterated Poisson bracket go through also for the scalar field reference fields φ^j. We just have to replace S^a_j by φ^a_j. For the benefit of the reader we have reviewed the proof in the appendix in section B. Using this result we obtain for the case that f is a scalar function, e.g. some function $g : \chi \mapsto \mathbb{R}$ on χ

$$\{K_{\beta_1}, g(x)\}_{(n)} = \big[\beta_1^{j_1}...\beta_1^{j_n} v_{j_1}...v_{j_n} \cdot g\big](x) \tag{302}$$

with $v_j \cdot g(x) = \varphi^a_j g_{,a}(x)$. Hence the spatially diffeomorphism invariant quantity for g is given by

$$O^{(1)}_{g,\{\varphi^j\}}(\sigma) = g + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \big[\sigma^{j_1} - \varphi^{j_1}\big]...\big[\sigma^{j_n} - \varphi^{j_n}\big] v_{j_1}...v_{j_n} \cdot g. \tag{303}$$

We have $v_j \cdot \varphi^k = \varphi^a_j \varphi^k_{,a} = \delta^k_j$. To see this, in eq. (831) in appendix B we calculated the action of the vector field v_k on $O^{(1)}_{g,\{\varphi^j\}}(\sigma)$. The result is given by

$$v_k \cdot O^{(1)}_{g,\{\varphi^j\}}(\sigma) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \beta_1^{j_1}...\beta_1^{j_n} \big[v_k \sigma^j\big] v_j v_{j_1}...v_{j_n} \cdot g. \tag{304}$$

As explained in the appendix we are allowed to choose any σ^j and a convenient choice is σ^j to be constant. This requires that φ^j is invertible for $j = 1, 2, 3$ which is an assumption entering the whole construction and means that $\varphi^j : \chi \mapsto \mathcal{S}$ can be understood as a diffeomorphism, where we denote with $\mathcal{S}$ the ***scalar reference field manifold***. Hence, for a scalar function g on χ

we therefore obtain the following explicit integral representation for the spatially diffeomorphism invariant expression

$$O^{(1)}_{g,\{\varphi^j\}}(\sigma) = \int\limits_{\chi} \mathrm{d}^3x \, \big|\det(\partial\varphi^j/\partial_x)\big| \delta(\varphi^j(x), \sigma^j) g(x). \tag{305}$$

Now as introduced in [26] for the quantities that are no scalars on χ we use the inverse map $(\varphi^j)^{-1} : \mathcal{S} \mapsto \chi$ to pull back tensors that become scalars on χ but tensors of same rank on $\mathcal{S}$, where we denote the physical space being the range of σ^j within $\mathcal{S}$. Explicitly, we construct for all variables that are not reference fields for c^{tot}_j using the abbreviation $J := |\det(\partial\varphi^j/\partial_x)|$ the following quantities

$$\varphi^0, \quad \pi_0/J, \quad q_{jk} = q_{ab}\varphi^a_j\varphi^b_k, \quad p^{jk} = p^{ab}\varphi^j_{,a}\varphi^k_{,b}/J, \tag{306}$$

where J is used to transform the scalar/tensor densities of weight one π_0 and p^{ab} into true scalars/tensors. The integral representations of the corresponding observables are then given by

$$\begin{aligned}
\widetilde{\varphi}^0 &:= O^{(1)}_{\varphi^0,\{\varphi^j\}}(\sigma) = \int\limits_{\chi} \mathrm{d}^3x \, \big|\det(\partial\varphi^j/\partial_x)\big| \delta(\varphi^j(x), \sigma^j)\varphi^0(x), \\
\widetilde{\pi}_0 &:= O^{(1)}_{\pi_0,\{\varphi^j\}}(\sigma) = \int\limits_{\chi} \mathrm{d}^3x \, \delta(\varphi^j(x), \sigma^j)\pi_0(x), \\
\widetilde{q}_{jk} &:= O^{(1)}_{q_{ab},\{\varphi^j\}}(\sigma) = \int\limits_{\chi} \mathrm{d}^3 \, \big|\det(\partial\varphi^j/\partial_x)\big| \delta(\varphi^j(x), \sigma^j)\varphi^a_j\varphi^b_k q_{ab}(x), \\
\widetilde{p}^{jk} &:= O^{(1)}_{p^{ab},\{\varphi^j\}}(\sigma) = \int\limits_{\chi} \mathrm{d}^3 \, \delta(\varphi^j(x), \sigma^j)\varphi^j_a\varphi^k_b p^{ab}(x),
\end{aligned} \tag{307}$$

where we will denote spatially diffeomorphism invariant quantities with a tilde. For the degrees of freedom that adopt the role of a reference field for c^{tot}_j we get

$$\begin{aligned}
\widetilde{\varphi}^j &= O^{(1)}_{\varphi^j,\{\varphi^j\}}(\sigma) = \Big[\alpha^{K_{\beta_1}}_{\beta_1}(\varphi^j)\Big]_{\alpha^{K_{\beta_1}}_t(\varphi^j)=\sigma^j} = \sigma^j = \int\limits_{\chi} \mathrm{d}^3 \, \big|\det(\partial\varphi^j/\partial_x)\big| \delta(\varphi^j(x), \sigma^j)\varphi^j(x), \\
\widetilde{\pi}_j &= O^{(1)}_{\pi_j,\{\varphi^j\}}(\sigma) = \int\limits_{\chi} \mathrm{d}^3 \, \big|\det(\partial\varphi^j/\partial_x)\big| \delta(\varphi^j(x), \sigma^j)\pi_j(x).
\end{aligned} \tag{308}$$

Thus, the spatially diffeomorphism invariant version of the constraints $\widetilde{c}^{\mathrm{tot}}$ and $\widetilde{c}^{\mathrm{tot}}_a$ become

$$\begin{aligned}
\widetilde{c}^{\mathrm{tot}} &= \widetilde{\pi}_0 + \widetilde{h}, \\
\widetilde{c}^{\mathrm{tot}}_j &= \widetilde{\pi}_j + \widetilde{h}_j = \widetilde{\pi}_j + \widetilde{c}^{\mathrm{geo}}_j - \widetilde{h}\widetilde{\varphi}^0_{,j} = \widetilde{\pi}_j - 2\widetilde{q}_{j\ell}D_k\widetilde{p}^{k\ell} - \widetilde{h}\widetilde{\varphi}^0_{,j},
\end{aligned} \tag{309}$$

where we used that

$$O^{(1)}_{\varphi^j_{,a}}(\sigma) = \int\limits_{\chi} \mathrm{d}^3x \big|\det(\partial\varphi^j/\partial_x)\big| \delta(\varphi^j(x), \sigma^j)\varphi^j_{,a}\varphi^a_k = \delta^j_k, \tag{310}$$

and likewise $O^{(1)}_{\varphi^a_{,j}}(\sigma) = \delta^k_j$ with

$$\begin{aligned}\widetilde{h} &= \frac{1}{1+\widetilde{\varphi}^0_{,j}\widetilde{\varphi}^0_{,k}\delta^{jk}} \times \Big(-\widetilde{c}^{\,\mathrm{geo}}_j\widetilde{\varphi}^0_{,k}\delta^{jk} \\ &+ \sqrt{\Big[\widetilde{c}^{\,\mathrm{geo}}_j\widetilde{\varphi}^0_{,k}\delta^{jk}\Big]^2 - \Big(1+\widetilde{\varphi}^0_{,j}\widetilde{\varphi}^0_{,k}\delta^{jk}\Big)\Big[2\sqrt{\det(\widetilde{q})}\widetilde{c}^{\,\mathrm{geo}} + \det(\widetilde{q})\widetilde{q}^{jk}\big(\widetilde{\varphi}^0_{,j}\widetilde{\varphi}^0_{,k}+\delta_{jk}\big) + \widetilde{c}^{\,\mathrm{geo}}_j\widetilde{c}^{\,\mathrm{geo}}_k\delta^{jk}\Big]}\Big), \\ \widetilde{c}^{\,\mathrm{geo}} &= \frac{1}{\sqrt{\det(\widetilde{q})}}\Big(\widetilde{q}_{j\ell}\widetilde{q}_{km} - \frac{1}{2}\widetilde{q}_{jk}\widetilde{q}_{\ell m}\Big)\widetilde{p}^{jk}\widetilde{p}^{\ell m} - \sqrt{\det(\widetilde{q})}R(\widetilde{q}).\end{aligned} \tag{311}$$

Next we will continue with constructing full observables that are also invariant under $\widetilde{c}^{\,\mathrm{tot}}$. As before we denote the smeared Hamiltonian constraint as

$$\widetilde{K}_{\beta_2} := \int_{\mathcal{S}} \mathrm{d}^3\sigma\, \beta_2 \widetilde{c}^{\,\mathrm{tot}}. \tag{312}$$

Then the observables are given by the power series

$$\begin{aligned}&O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{f}(\sigma),\widetilde{\varphi}^0}(\sigma)(\tau) \\ &= \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Big[\{\widetilde{K}_{\beta_2},\widetilde{f}\}_{(n)}\Big]_{\beta_2=\tau-\widetilde{\varphi}^0} \\ &= \widetilde{f}(\sigma) + \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\int_{\mathcal{S}}\mathrm{d}^3\sigma'_1(\tau-\widetilde{\varphi}^0(\sigma'_1))...\int_{\mathcal{S}}\mathrm{d}^3\sigma'_n(\tau-\widetilde{\varphi}^0(\sigma'_n))\{\widetilde{c}^{\,\mathrm{tot}}(\sigma'_1),...\{\widetilde{c}^{\,\mathrm{tot}}(\sigma'_n),\widetilde{f}(\sigma)\}...\}.\end{aligned} \tag{313}$$

Again we want $\int \mathrm{d}^3\sigma(\tau-\widetilde{\varphi}^0(\sigma))\widetilde{h}(\sigma)$ to be spatially diffeomorphism invariant. This requires a constant τ. We will denote full observables by capital letters, explicitly

$$\begin{aligned}Q_{jk}(\sigma,\tau) &:= O_{q_{ab},\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{q}_{jk}(\sigma),\widetilde{\varphi}^0}, \\ P^{jk}(\sigma,\tau) &:= O_{p^{ab},\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{p}^{jk}(\sigma),\widetilde{\varphi}^0}, \\ \Pi_0(\sigma,\tau) &:= O_{\pi_0,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{\pi}_0(\sigma),\widetilde{\varphi}^0}, \\ \Pi_j(\sigma,\tau) &:= O_{\pi_j,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{\pi}_j(\sigma),\widetilde{\varphi}^0}.\end{aligned} \tag{314}$$

Note that Π_0 and Π_j are no independent observables because using the constraints in eq. (299) these can be expressed in terms of Q^{jk} and P_{jk}. Furthermore we have

$$O_{\varphi^0,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = \tau \quad \text{and} \quad O_{\varphi^j,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = \sigma^j. \tag{315}$$

7.4 Step 2: Dynamics encoded in the Physical Hamiltonian

Likewise to the dust case in [26] this power series for $O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau)$ cannot be written down in closed form. However, what is more important is that we know an explicit form of the physical Hamiltonian $\mathbf{H}_{\mathrm{phys}}$ generating the evolution with respect to the physical time τ. Therefore, we could derive equations of motion for $O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau)$. Solving these equations yields a possibility to obtain an explicit expression for the observables. When choosing dust fields as reference fields it could be shown that $\mathbf{H}_{\mathrm{phys}}$ is the (physical) space integral over $\mathcal{S}$ of the observable associated with the function h in c^{tot}, see [26] for more details. The proof that $\mathbf{H}_{\mathrm{phys}}$ generates τ- evolution uses the property that c^{tot} deparametrizes for the dust reference fields. Nevertheless, as we will show now also in the scalar field case where deperametrization is not present $\mathbf{H}_{\text{phys}}$ can be expressed as the integral over the observable associated with h. Let us consider phase space functions f that are independent of the reference field degrees of freedom used for c^{tot} that is f is not allowed to depend on φ^0 and/or π_0. Then by considering the explicit power series for observables in eq. (313) we have

$$
\begin{aligned}
&\frac{d}{d\tau}O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = \frac{d}{d\tau}O^{(2)}_{\widetilde{f}(\sigma),\widetilde{\varphi}^0(\sigma)}(\tau) \qquad (316)\\
&= \sum_{n=1}^{\infty}\frac{(-1)^n}{(n-1)!}\int_{\mathcal{S}} d^3\sigma'_1\ldots\int_{\mathcal{S}} d^3\sigma'_n\{\widetilde{c}^{\text{tot}}(\sigma'_1),\ldots\{\widetilde{c}^{\text{tot}}(\sigma'_n),\widetilde{f}(\sigma)\}\ldots\}(\tau-\widetilde{\varphi}^0(\sigma'_2))\ldots(\tau-\widetilde{\varphi}^0(\sigma'_n))\\
&= -\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_{\mathcal{S}} d^3\sigma'_1\ldots\int_{\mathcal{S}} d^3\sigma'_n\{\widetilde{c}^{\text{tot}}(\sigma'_1),\ldots\{\widetilde{c}^{\text{tot}}(\sigma'_n),\ldots\\
&\qquad\qquad -\{\int_{\mathcal{S}} d^3\sigma'\widetilde{c}^{\text{tot}}(\sigma'),\widetilde{f}(\sigma)\}\ldots\}(\tau-\widetilde{\varphi}^0(\sigma'_1))\ldots(\tau-\widetilde{\varphi}^0(\sigma'_n))\\
&= -O_{\{\int_{\mathcal{S}} d^3\sigma'\widetilde{c}^{\text{tot}}(\sigma'),\widetilde{f}(\sigma)\},\widetilde{\varphi}^0(\sigma)}(\tau)\\
&= -O_{\{\int_{\mathcal{S}} d^3\sigma'\widetilde{h}(\sigma'),\widetilde{f}(\sigma)\},\widetilde{\varphi}^0(\sigma)}(\tau)\\
&= -O_{\{\int_{\mathcal{S}} d^3\sigma'\widetilde{h}(\sigma'),\widetilde{f}(\sigma)\}^*,\widetilde{\varphi}^0(\sigma)}(\tau)\\
&= -\{O_{O^{(1)}_{\int_{\mathcal{X}} d^3x' h(x'),\varphi^j}(\sigma),\widetilde{\varphi}^0(\sigma)}(\tau),O_{O^{(1)}_{f,\varphi^j}(\sigma),\widetilde{\varphi}^0(\sigma)}(\tau)\}^*\\
&= \{O_{\int_{\mathcal{X}} d^3x' h(x'),\{\varphi^0,\varphi^j\}}(\tau),O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau)\}\\
&= -\{O_{\int_{\mathcal{S}} d^3\sigma'\widetilde{h}(\sigma'),\{\varphi^0,\varphi^j\}}(\tau),O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau)\}\\
&= -\{\int_{\mathcal{S}} d^3\sigma' O_{h,\{\varphi^0,\varphi^j\}}(\sigma'\tau),O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau)\} = \{\int_{\mathcal{S}} d^3\sigma' H(\sigma',\tau),O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau)\}\\
&= -\{\mathbf{H}_{\text{phys}}(\tau),O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau)\} = \{O_{f,\{\varphi^0,\varphi^j\}}(\sigma,\tau),\mathbf{H}_{\text{phys}}(\tau)\}.
\end{aligned}
$$

In the third line we used that $\widetilde{c}^{\text{tot}}(\sigma)$ mutually commute and in the fifth line that f is by assumption independent of φ^0 that allows us to replace $\widetilde{c}^{\text{tot}}$ by $\widetilde{h}$. Furthermore we could use the Poisson bracket instead of the corresponding Dirac bracket because $\widetilde{f}$ (by assumption) does not depend on the reference field momentum π_0, compare section 5. Consequently, all terms in the Dirac bracket additional to the Poisson bracket vanish. The Dirac bracket here has the following form for the spatial diffeomorphism invariant quantities

$$
\{\widetilde{f},\widetilde{f}'\}^* := \{\widetilde{f},\widetilde{f}'\} - \int_{\mathcal{S}} d^3\sigma\left(\{\widetilde{f},\widetilde{c}^{\text{tot}}(\sigma)\}\{\widetilde{f}',\widetilde{\varphi}^0(\sigma)\} - \{\widetilde{f}',\widetilde{c}^{\text{tot}}(\sigma)\}\{\widetilde{f},\widetilde{\varphi}^0(\sigma)\}\right) \qquad (317)
$$

and for the unreduced case

$$
\{f,f'\}^* := \{f,f'\} - \int_{\mathcal{X}} d^3x\sum_{J=0}^{3}\left(\{f,c^{\text{tot}}_J(x)\}\{f',\varphi^J(x)\} - \{f',c^{\text{tot}}_J(x)\}\{f,\varphi^J(x)\}\right) \qquad (318)
$$

with $c_0^{\rm tot} := c^{\rm tot}$. In the last before the last line in eq. (316) we used the linearity of the observable map and introduced the abbreviation $H(\sigma,\tau) := O_h(\sigma,\tau)$. Thus, the physical Hamiltonian in case of the Klein-Gordon scalar field reference field is given by the following expression

$$\mathbf{H}_{\rm phys} := \int\limits_{\mathcal{S}} d^3\sigma\, O^{(2)}_{\widetilde{h}(\sigma),\widetilde{\varphi}^0}(\sigma,\tau) = \int\limits_{\mathcal{S}} d^3\sigma\, H(\sigma,\tau), \tag{319}$$

here we denote the (full) observable associated to h according to our notation by H and the latter is explicitly given by

$$H(\sigma) = \sqrt{-\Big(2\sqrt{\det(Q)}C^{\rm geo} + \det(Q)Q^{jk}\delta_{jk} + \delta^{jk}C^{\rm geo}_j C^{\rm geo}_k\Big)} \tag{320}$$

and does not depend on the physical time τ where

$$\begin{aligned} C^{\rm geo} &:= \frac{1}{\sqrt{\det(Q)}}\Big(Q_{j\ell}Q_{km} - \frac{1}{2}Q_{jk}Q_{\ell m}\Big)P^{jk}P^{\ell} - \sqrt{\det(Q)}R(Q) + 2\sqrt{\det(Q)}\Lambda, \\ C^{\rm geo}_j &:= -2Q_{j\ell}D_k P^{k\ell}. \end{aligned} \tag{321}$$

The reason why H includes less terms than $\widetilde{h}$ in eq. (311) and looks less complicated is that all terms involving spatial derivatives of the reference field $\widetilde{\varphi}^0$ can be dropped because $O^{(2)}_{\widetilde{\varphi}^0_{,j},\widetilde{\varphi}^0}(\sigma,\tau) = d\tau/d\sigma^j = 0$. A side effect of this is that $\mathbf{H}_{\rm phys}$ although involving still explicit reference field variable dependence $\widetilde{\varphi}^0$, is nevertheless a time independent Hamiltonian since only derivative terms occur. However, the additional explicit dependence on the reference fields $\widetilde{\varphi}^j$ survives because their derivatives give a contribution in terms of Kronecker deltas. From the first impression it sound astonishing that although we started with a full covariant theory, we end up with a physical Hamiltonian that looks not covariantly due to the occurring Kronecker deltas. Though, we should keep in mind that the index j in the equation above refers to the label of the scalar reference fields and is no spatial index of a space-time index. Thus, the non-covariance of the physical Hamiltonian refers to the manifold $\mathcal{S}$ associated to the spatial reference fields φ^j and there is no guarantee that $\mathbf{H}_{\rm phys}$ might be covariant there even if we start with a covariant action on χ.
Furthermore in contrast to the deparametrized dust case here we cannot conclude from the fact that the $c^{\rm tot}$'s mutually commute that also the h's do. For this reason it is more complicated to understand in the scalar field case what precise symmetries $\mathbf{H}_{\rm phys}$ possesses. This will be discussed more in detail in future work.

7.5 Step 3: Reduced Phase Space Quantization

Finally, we would like to complete the quantization program and find a representation of the observables algebra whose non-vanishing Poisson brackets are given by

$$\{Q^{jk}(\sigma,\tau), P_{\ell m}(\widetilde{\sigma},\tau)\} = \delta^j_\ell \delta^k_m \delta^{(3)}(\sigma,\widetilde{\sigma}). \tag{322}$$

For the reason that we want to apply the quantization used in Loop Quantum Gravity, we formulate the geometry phase space in terms of su(2) connections and canonically conjugate fields (A^A_a, E^a_A), i.e. as Ashtekar variables, rather than in terms of the ADM variables Q^{jk}, P_{jk}, where A is a su(2) index. This describes the geometrical sector of the phase space as a SU(2) Yang-Mills theory. As mentioned in section 2.4, as a consequence we obtain next to the Hamiltonian and spatial diffeomorphism constraint the so-called SU(2) Gauss constraint on the (extended) phase space. If we perform a symplectic reduction with respect to the Gauss constraint we get back the usual ADM phase space. Now in the context of Ashtekar variables the observables constructed in section 7.3 describe a partially reduced phase space (only with respect to the Hamiltonian and spatial diffeomorphism constraint) on which we still have to solve the Gauss constraint given by

$$G_A := \partial_j E^j_A + \epsilon_{AB}^{C} A^B_j E^j_C. \tag{323}$$

The introduction of Ashtekar variables allows to rewrite general relativity in terms of the language of gauge fields and this suggests to formulate the theory in terms of holonomies along one dimensional paths and electric fluxes through two dimensional surfaces, likewise to the case when one applies Dirac quantization in unreduced Loop Quantum Gravity as displayed in part II. For the unreduced case a uniqueness result [95, 134] showing that cyclic representations of the holonomy – flux algebra which implement a unitary representation of the spatial diffeomorphism gauge group Diff(χ) are unique and are unitarily equivalent to the Ashtekar – Isham – Lewandowski representation [107, 111]. In our case, that considers the (partially) reduced phase space, we do not have the diffeomorphism gauge group but rather a diffeomorphism symmetry group Diff($\mathcal{S}$) of the physical Hamiltonian $\mathbf{H}_{\rm phys}$. This is physical input enough to also insist on cyclic Diff($\mathcal{S}$) covariant representations and correspondingly, like in [5] we can copy the uniqueness result. Hence, we choose the background independent and active diffeomorphism covariant Hilbert space representation of Loop Quantum Gravity that becomes the representation of the physical Hilbert space here. Thus, $\mathcal{H}_{\rm phys} = L_2(\bar{\mathcal{A}}, \mu_0)$ can be understood as the space of square integrable function over the set of generalized connections with respect to Ashtekar-Lewandowski measure μ_0, for more details and a pedagogical introduction, see part II section 2.2 and for instance [6, 9, 10, 12, 13, 135, 136] and references therein. We solve the remaining Gauss constraint by simply restricting to the gauge invariant sector of that Hilbert space. This can be achieved by choosing appropriate intertwiners for the vertices of the so-called spin network functions that provide an orthornomal basis in $\mathcal{H}_{\rm phys}$. For more details see also [5] and part II section 2.4.
As mentioned earlier we are only interested in those representations that also allow to implement the physical Hamiltonian $\mathbf{H}_{\rm phys}$ as a well defined operator. However, looking at the particular form of the physical Hamiltonian density in eq. (320), we realize that it is exactly this point where the ***reduced phase space quantization cannot be performed***. Let us explain this in detail: Due to the fact that in the Loop Quantum Gravity representation used for $\mathcal{H}_{\rm phys}$ the spatial diffeomorphisms are not implemented weakly continuously, only finite diffeomorphism exists at the quantum level but the associated infinitesimal generators cannot be defined as operators on $\mathcal{H}_{\rm phys}$, see for example part II section 2.4. In our model this carries directly over to $C^{\rm geo}_j$. As a consequence the expression $\delta^{jk} C^{\rm geo}_j C^{\rm geo}_k$ under the square root cannot be quantized and this implies that the physical Hamiltonian $\mathbf{H}_{\rm phys}$ cannot be implemented as a well defined operator on $\mathcal{H}_{\rm phys}$. This shows that the four Klein-Gordon scalar fields model is an example for a model where Dirac quantization and reduced quantization yield very different results. In case we would use this model and apply Dirac quantization we would meet no technical problem in implementing the constraint operators on the kinematical Hilbert space that also involve the contribution from the Klein-Gordon scalar fields. Therefore, a formulation of the Quantum Einstein Equations in the context of Dirac quantization would be possible, although the final physical Hilbert space would still need to be derived. However, in the case of reduced quantization, we are able to construct the physical Hilbert space $\mathcal{H}_{\rm phys}$, but then on $\mathcal{H}_{\rm phys}$ the dynamics encoded in the physical Hamiltonian cannot be formulated as a well defined operator. Therefore, the quantization program cannot be completed in the reduced case. This implies that four Klein-Gordon scalar fields do not provide an appropriate set of reference fields in order to obtain a reduced phase space quantization of general relativity.

Let us close this section with a few remarks.

1. One could ask the question why such issues are not present in any of the other currently available reference matter models. The reason for this is that in all current available models the generator C_j^{geo} occurs only in the combination $Q^{jk}C_j^{\mathrm{geo}}C_k^{\mathrm{geo}}$ and it is exactly this combination that can again be quantized in the usual Loop Quantum Gravity representation [5] used for $\mathcal{H}_{\mathrm{phys}}$ here.
2. In [137] a lot of progress was made to formulate an operator that corresponds to infinitesimal spatial diffeomorphisms at the classical level. However, because this work requires a particular phase space dependent form of the shift vector, the techniques developed there cannot be applied here in order to find a suitable quantization of $\mathbf{H}_{\mathrm{phys}}$ on $\mathcal{H}_{\mathrm{phys}}$.
3. One could take the point of view that this negative result does only occur because we require the theory to be quantizable within the representation used in Loop Quantum Gravity. However, if we drop this requirement and consider for instance Fock quantization, then we could not implement the original constraints and quantities like the volume operator as well defined operators on Fock space. Therefore the situation is even worse in that case.

In summary, we conclude that the four Klein-Gordon scalar fields model cannot be used as a natural extension of the APS-model [24] and the one scalar field model [1] to obtain the corresponding reduced quantum theories associated with these models. In section 9 we will demonstrate that a slight generalization of the four Klein-Gordon scalar fields model is sufficient enough to get a model for which the dynamics can be implemented and thus the reduced phase space quantization program can be completed but before that we will consider a more general case.

8 Generalized Model with four Klein-Gordon Scalar Fields

The introduction to this section is similar to an introduction to a section in [130], however in this section we consider first an additional model that is not discussed in [130]. We saw that the combination of the standard action of four Klein-Gordon scalar fields with the Einstein-Hilbert action describing the gravitational field results on the level of observables into a physical Hamiltonian which cannot be quantized on $\mathcal{H}_{\mathrm{phys}}$ in the usual LQG representation due to the fact that an operator for the generator C_j^{geo} of infinitesimal diffeomorphisms on $\mathcal{H}_{\mathrm{kin}}$ in LQG does not exist. In a second ansatz we want to extend the former model with four Klein-Gordon scalar fields in order to obtain a model that is suitable for completing the quantization program in the reduced case. The seminal models [27, 132] have a common property, namely that at first they introduce more than the necessary four scalar fields in addition to general relativity. It turns out that then these models describe a system with second class constraints. A symplectic reduction with respect to the second class constraints results in a first class model with only four additional scalar fields. For the generalization of the four Klein-Gordon scalar fields model we want to follow a similar way. We first introduce six additional scalar fields which will later in section 9, after a further simplification, reduce to three additional scalar fields in such a way that the final physical Hamiltonian can be quantized on $\mathcal{H}_{\mathrm{phys}}$. The model we want to consider contains a modified Klein-Gordon action. It can be described by the following total action

$$\begin{aligned} S[g,\varphi^0,\varphi^j,M_{ij}] &= \int\limits_M \mathrm{d}^4Y\sqrt{g}R^{(4)} - \frac{1}{2}\int\limits_M \mathrm{d}^4Y\sqrt{g}g^{\mu\nu}\varphi^0_{,\mu}\varphi^0_{,\nu} - \frac{1}{2}\int\limits_M \mathrm{d}^4Y\sqrt{g}M_{ij}g^{\mu\nu}\varphi^i_{,\mu}\varphi^j_{,\nu} \qquad (324)\\ &= S^{\mathrm{geo}} + S^{\varphi^0} + S^{\varphi^j}, \end{aligned}$$

where we assume that the indices μ, ν run from 0 to 3 and M is a 3x3 matrix with entries M_{ij} whereas the indices i,j run from 1 to 3 and we sum over repeated indices here. Note that we also could have considered a model with a 4x4 matrix with entries $M_{IJ},\ I,J=0,\ldots,3$. However, then the reference field for the Hamiltonian constraint would no longer be a standard Klein-Gordon field and since we want to compare our model to the one in [1], we will only work with a spatial matrix here. In principle we have introduced 9 new degrees of freedom sitting in a not further restricted arbitrary matrix M in three dimensions. In the course of this part we will put further restrictions on this matrix which will reduce the number of independent degrees of freedom. In this respect the first assumption we make is that M is a symmetric matrix, that is $M_{ij}=M_{ji}$, which reduces the number of degrees of freedom from 9 to 6. Again we perform the ADM split and define $\varphi^I_n := n^\mu \varphi^I_{,\mu}$, $I=0,\ldots,3$ with $n^\mu = \frac{1}{n}[Y^\mu_{,t} - n^a Y^\mu_{,a}]$ and $\varphi^I_{,a} := Y^\mu_{,a}\varphi^I_{,\mu}$ then our modified Klein-Gordon action in the ADM frame reads

$$S^{\varphi^0} + S^{\varphi^j} = +\frac{1}{2}\int\limits_{\mathbb{R}} \mathrm{d}t \int\limits_{\chi} \mathrm{d}^3x\, n\,\sqrt{q}\left(\left[\varphi^0_n\right]^2 - q^{ab}\varphi^0_{,a}\varphi^0_{,b} + M_{ij}\varphi^i_n\varphi^j_n - M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b}\right). \tag{325}$$

8.1 Total Action in Canonical Form

Analogous to the previous case of four standard Klein-Gordon scalar fields we need to calculate the canonically conjugate momenta of the total action $S^{\text{geo}} + S^{\varphi^0} + S^{\varphi^j}$, where S^{geo} denotes the Einstein-Hilbert action, to bring the action into canonical form. In the following again a dot denotes the partial derivative with respect to the time parameter t, that is $\dot{\varphi}^I := \varphi^I_{,t}$ with $I=0,\ldots,3$.

The canonically conjugate momentum corresponding to the scalar field φ^0 is given by

$$\begin{aligned}\pi_0 := \frac{\delta S}{\delta\dot{\varphi}^0} &= \int\limits_{\mathbb{R}} \mathrm{d}t \int\limits_{\chi} \mathrm{d}^3x\, n\,\sqrt{q}\varphi^0_n \frac{\delta\varphi^0_n}{\delta\dot{\varphi}^0} \\ &= \int\limits_{\mathbb{R}} \mathrm{d}t \int\limits_{\chi} \mathrm{d}^3x\, n\,\sqrt{q}\varphi^0_n \frac{1}{n}\delta^{(4)}(x,y) = \sqrt{q}\varphi^0_n.\end{aligned} \tag{326}$$

For the conjugate momenta of the spatial scalar fields φ^j we obtain

$$\begin{aligned}\pi_j := \frac{\delta S}{\delta\dot{\varphi}^j} &= \frac{1}{2}\int\limits_{\mathbb{R}} \mathrm{d}t \int\limits_{\chi} \mathrm{d}^3x\, n\,\sqrt{q}\left(M_{ik}\frac{\delta\varphi^i_n}{\delta\dot{\varphi}^j}\varphi^k_n + M_{ik}\varphi^i_n\frac{\delta\varphi^k_n}{\delta\dot{\varphi}^j}\right) \\ &= \frac{1}{2}\int\limits_{\mathbb{R}} \mathrm{d}t \int\limits_{\chi} \mathrm{d}^3x\,\sqrt{q}\left(M_{ik}\delta^i_j\varphi^k_n + M_{ik}\varphi^i_n\delta^k_j\right)\delta^{(4)}(x,y) \\ &= \frac{1}{2}\sqrt{q}\left(M_{jk}\varphi^k_n + M_{ij}\varphi^i_n\right) = \sqrt{q}M_{jk}\varphi^k_n.\end{aligned} \tag{327}$$

In the last step we used that we assume the matrix M to be symmetric, that is $M_{kj}=M_{jk}$ and changed the index i into k, since here we sum over repeated indices. In this case we are in a different situation compared to our first approach with the four standard Klein-Gordon fields in section 7: π_0 can still be solved for its velocity $\dot{\varphi}^0$ but the π_j could only be solved for $\dot{\varphi}^j$, if we assumed that M is also invertible due to the summation over k. Therefore, for a non-invertible matrix M a ***new primary constraint*** arises which we denote as Φ_j and define by

$$\Phi_j := \pi_j - \sqrt{q}M_{jk}\varphi^k_n = 0, \tag{328}$$

for a symmetric matrix M. We consider the entries M_{ij} of the matrix M as dynamical variables, so we also need to calculate their canonically conjugate momenta

$$\Pi^{ij} := \Lambda^{ij} := \frac{\delta S}{\delta \dot{M}_{ij}} = 0. \tag{329}$$

As before the canonically conjugate momenta corresponding to lapse n and shift n^a are

$$p := z := \frac{\delta S}{\delta \dot{n}} = 0, \tag{330}$$

$$p_a := z_a := \frac{\delta S}{\delta \dot{n}_a} = 0. \tag{331}$$

In summary Φ_j, Λ^{ij}, z, z_a are primary constraints, since they cannot be solved for their corresponding velocities. Performing the Legendre transformation yields to the total action in canonical form

$$\begin{aligned} S = &\int_{\mathbb{R}} \mathrm{d}t \int_{\chi} \mathrm{d}^3x \, (\frac{1}{\kappa}\dot{q}_{ab}p^{ab} + \dot{\varphi}^0\pi_0 + \dot{\varphi}^j\pi_j + \dot{n}p + \dot{n}_a p_a + \dot{M}_{ij}\Pi^{ij}) \\ &- \int_{\mathbb{R}} \mathrm{d}t \int_{\chi} \mathrm{d}^3x \, h_{\text{primary}} \end{aligned} \tag{332}$$

and h_{primary} is given by

$$h_{\text{primary}} = \nu z + \nu_a z^a + \rho^j \Phi_j + \mu_{ij}\Lambda^{ij} + \frac{1}{\kappa}\dot{q}_{ab}p^{ab} - \mathcal{L}_{\text{geo}} + \dot{\varphi}^0\pi_0 + \dot{\varphi}^j\pi_j - \mathcal{L}_{\varphi}. \tag{333}$$

The term $\frac{1}{\kappa}\dot{q}_{ab}p^{ab} - \mathcal{L}_{\text{geo}}$ gives rise to the geometric part of the Hamiltonian and diffeomorphism constraints c^{geo} and c^{geo}_a as already displayed in [26] and above in section 7.1. From the term $\dot{\varphi}^0\pi_0 + \dot{\varphi}^j\pi_j - \mathcal{L}_{\varphi}$ we determine the part of the constraints belonging to the four Klein-Gordon fields which leads to

$$\begin{aligned} &\dot{\varphi}^0\pi_0 + \dot{\varphi}^j\pi_j - \mathcal{L}_{\varphi} \\ &= \dot{\varphi}^0\pi_0 - \frac{1}{2}n\sqrt{q}\left(\left[\varphi^0_n\right]^2 - q^{ab}\varphi^0_{,a}\varphi^0_{,b} + M_{ij}\varphi^i_n\varphi^j_n - M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b}\right) + \dot{\varphi}^j\pi_j \\ &= \frac{n}{2}\sqrt{q}\left[\frac{\pi_0^2}{q} + q^{ab}\varphi^0_{,a}\varphi^0_{,b} - M_{ij}\varphi^i_n\varphi^j_n + M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b}\right] + n^a\,\pi_0\varphi^0_{,a} + n\,\pi_j\varphi^j_n + n^a\pi_j\varphi^j_{,a} \\ &= \frac{n}{2}\sqrt{q}\left[\frac{\pi_0^2}{q} + q^{ab}\varphi^0_{,a}\varphi^0_{,b}\right] + n^a\,\pi_0\varphi^0_{,a} + n^a\pi_j\varphi^j_{,a} + n\,\pi_j\varphi^j_n - \frac{n}{2}\sqrt{q}\left[M_{ij}\varphi^i_n\varphi^j_n - M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b}\right] \\ &=: n\,c^{\varphi^0} + n^a\left(c^{\varphi^0}_a + c^{\varphi^j}_a\right) + n\pi_j\varphi^j_n - \frac{n}{2}\sqrt{q}\left[M_{ij}\varphi^i_n\varphi^j_n - M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b}\right] \\ &=: n\,c^{\varphi^0} + n^a\,c^{\varphi}_a + \frac{n}{2}\varphi^j_n\left[2\pi_j - \sqrt{q}M_{ij}\varphi^i_n\right] + \frac{n}{2}\sqrt{q}M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b} \\ &= n\,c^{\varphi^0} + n^a\,c^{\varphi}_a + \frac{n}{2}\varphi^j_n\pi_j + \frac{n}{2}\sqrt{q}M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b} + \frac{n}{2}\varphi^j_n\Phi_j, \end{aligned} \tag{334}$$

where we used that $\pi_0 = \sqrt{q}\varphi^0_n$ and we can solve for the velocities $\dot{\varphi}^0$ according to

$$\varphi^0_n = \frac{1}{n}(\dot{\varphi}^0 - n^a\varphi^0_{,a}) \Leftrightarrow \dot{\varphi}^0 = n\varphi^0_n + n^a\varphi^0_{,a} = n\frac{\pi_0}{\sqrt{q}} + n^a\varphi^0_{,a}, \tag{335}$$

but we cannot solve for the velocity $\dot{\varphi}^j$ which therefore stays

$$\dot{\varphi}^j = n\varphi^j_n + n^a\varphi^j_{,a}. \tag{336}$$

Notice that from the last line in eq. (334) we see that we can consider φ^j_n as a Lagrange multiplier, since Φ_j is a primary constraint.

By defining $c^{\text{tot},0} := c^{\text{geo}} + c^{\varphi^0}$ and $c^{\text{tot}}_a := c^{\text{geo}}_a + c^{\varphi}_a = c^{\text{geo}}_a + c^{\varphi^0}_a + c^{\varphi^j}_a$ we can write the primary Hamiltonian as

$$\begin{aligned} H_{\text{primary}} &= \int\limits_\chi \mathrm{d}^3x\, h_{\text{primary}} \qquad (337)\\ &= \int\limits_\chi \mathrm{d}^3x \left(\nu z + \nu^b z_b + \rho^j\Phi_j + \mu_{ij}\Lambda^{ij} + nc^{\text{tot},0} + n^b c^{\text{tot}}_b + \frac{n}{2}\varphi^j_n\pi_j + \frac{n}{2}\sqrt{q}M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b} + \frac{n}{2}\varphi^j_n\Phi_j\right). \end{aligned}$$

Finally, the action in canonical form becomes

$$\begin{aligned} &S[q_{ab}, p^{ab}, n, p, n^a, p_a, \varphi^0, \pi_0, \varphi^j, \pi_j, M_{ij}, \Pi^{ij}] \qquad (338)\\ &= \int\limits_{\mathbb{R}} \mathrm{d}t \int\limits_\chi \mathrm{d}^3x \left(\frac{1}{\kappa}\dot{q}_{ab}p^{ab} + \dot{\varphi}^0\pi_0 + \dot{\varphi}^j\pi_j + \dot{n}p + \dot{n}^a p_a + \dot{M}_{ij}\Pi^{ij} - h_{\text{primary}}\right) \end{aligned}$$

with primary constraints

$$z := p, \quad z_a := p_a, \quad \Phi_j := \pi_j - \sqrt{q}M_{jk}\varphi^k_n, \quad \Pi^{ij} := \Lambda^{ij}$$

and we defined that

$$c^{\text{tot},0} := c^{\text{geo}} + c^{\varphi^0}, \quad c^{\text{tot}}_a := c^{\text{geo}}_a + c^{\varphi}_a$$

with

$$\begin{aligned} \kappa c^{\text{geo}} &= \frac{1}{\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right)p^{ab}p^{cd} - \sqrt{q}R^{(3)}, \qquad (339)\\ c^{\varphi^0} &= \frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b},\\ \kappa c^{\text{geo}}_a &= -2q_{ac}D_b p^{bc},\\ c^{\varphi}_a &= \pi_0\varphi^0_{,a} + \pi_j\varphi^j_{,a}. \end{aligned}$$

8.2 Constraint Stability Analysis

In the following we need to perform the constraint stability analysis in order to check whether the primary constraints are stable under time evolution with respect to H_{primary} or not. The non-vanishing Poisson brackets on the phase space are given by

$$\begin{aligned} \{q_{cd}(x), p^{ab}(y)\} &= \kappa\delta^a_{(c}\delta^b_{d)}\delta^{(3)}(x,y), \qquad (340)\\ \{n(x), p(y)\} &= \delta^{(3)}(x,y),\\ \{n^a(x), p_b(y)\} &= \delta^a_b\delta^{(3)}(x,y),\\ \{\varphi^0(x), \pi_0(y)\} &= \delta^{(3)}(x,y),\\ \{\varphi^j(x), \pi_k(y)\} &= \delta^j_k\delta^{(3)}(x,y),\\ \{M_{ij}(x), \Pi^{k\ell}(y)\} &= \delta^k_{(i}\delta^\ell_{j)}\delta^{(3)}(x,y). \end{aligned}$$

We need to calculate the Poisson brackets

$$
\begin{aligned}
\dot{z} &= \{z, H_{\text{primary}}\} = \{p, H_{\text{primary}}\}, \\
\dot{z}_a &= \{z_a, H_{\text{primary}}\} = \{p_a, H_{\text{primary}}\}, \\
\dot{\Lambda}^{ij} &= \{\Lambda^{ij}, H_{\text{primary}}\} = \{\Pi^{ij}, H_{\text{primary}}\}, \\
\dot{\Phi}_j &= \{\Phi_j, H_{\text{primary}}\} = \{\pi_j - \sqrt{q} M_{jk}\varphi^k_n, H_{\text{primary}}\}.
\end{aligned} \tag{341}
$$

After a tedious calculation which is displayed in detail in appendix D, we find that:

$$
\begin{aligned}
\dot{z} &= -\frac{1}{n}\rho^k \sqrt{q} M_{k\ell}\varphi^\ell_n - c^{\text{tot},0} - \frac{1}{2}\sqrt{q} M_{ij} q^{ab}\varphi^i_{,a}\varphi^j_{,b} - \frac{1}{2}\varphi^j_n \pi_j, \\
\dot{z}_a &= -\rho^k \sqrt{q} M_{k\ell}\frac{1}{n}\varphi^\ell_{,a} - c^{\text{tot}}_a + \frac{1}{2}\varphi^j_{,b}\pi_j + \frac{1}{2}\varphi^j_{,a}\Phi_j - \frac{1}{2}\varphi^j_n \sqrt{q} M_{j\ell}\varphi^\ell_{,a}, \\
\dot{\Lambda}^{ij} &= \rho^i \sqrt{q}\varphi^j_n + \frac{n}{2}\sqrt{q}\left(\varphi^i_n\varphi^j_n - q^{ab}\varphi^i_{,a}\varphi^j_{,b}\right), \\
\dot{\Phi}_j &= \nu\sqrt{q} M_{jk}\frac{1}{n}\varphi^k_n + \nu^b \sqrt{q} M_{jk}\frac{1}{n}\varphi^k_{,b} + \rho^k\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + 2\rho^k_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] \\
&\quad - \mu_{jk}\sqrt{q}\varphi^k_n + \frac{n}{2}M_{jk}\varphi^k_n q_{ab}p^{ab} + \sqrt{q}M_{jk}\varphi^k_n\left(-n^a_{,a} + n^a q_{ac} D_b q^{bc}\right) \\
&\quad + \left[\frac{1}{2}n^a\pi_j\right]_{,a} + \left[n\sqrt{q}q^{ab}M_{jk}\varphi^k_{,a}\right]_{,b} \\
&\quad + \left[\frac{n}{2}\varphi^k_n\right]\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + \left[\frac{n}{2}\varphi^k_n\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] - \left[\frac{n}{2}\Phi_j n^a\right]_{,a}.
\end{aligned} \tag{342}
$$

We see that for a symmetric matrix M we will generate new secondary constraints which are quite complicated due to the fact that we cannot solve for the velocities of the φ^j fields. Since we are only interested in finding a quantizable model including four Klein-Gordon scalar fields, we will make some further assumptions about the matrix M in section 9. We will see that this will work out to obtain a quantizable model, where we can solve for the velocities $\dot{\varphi}^j$.

We can compare the model here and in section 9 by choosing the Lagrange multiplier $\rho^k = 0$ which gives rise to

$$
\begin{aligned}
\dot{z} &= -c^{\text{tot},0} - \frac{1}{2}\sqrt{q} M_{ij} q^{ab}\varphi^i_{,a}\varphi^j_{,b} - \frac{1}{2}\varphi^j_n \pi_j, \\
\dot{z}_a &= -c^{\text{tot}}_a + \frac{1}{2}\varphi^j_{,b}\pi_j + \frac{1}{2}\varphi^j_{,a}\Phi_j - \frac{1}{2}\varphi^j_n \sqrt{q} M_{j\ell}\varphi\ell_{,a}, \\
\dot{\Lambda}^{ij} &= \frac{n}{2}\sqrt{q}\left(\varphi^i_n\varphi^j_n - q^{ab}\varphi^i_{,a}\varphi^j_{,b}\right), \\
\dot{\Phi}_j &= \nu\sqrt{q} M_{jk}\frac{1}{n}\varphi^k_n + \nu^b \sqrt{q} M_{jk}\frac{1}{n}\varphi^k_{,b} \\
&\quad - \mu_{jk}\sqrt{q}\varphi^k_n + \frac{n}{2}M_{jk}\varphi^k_n q_{ab}p^{ab} + \sqrt{q}M_{jk}\varphi^k_n\left(-n^a_{,a} + n^a q_{ac} D_b q^{bc}\right) \\
&\quad + \left[\frac{1}{2}n^a\pi_j\right]_{,a} - \varphi^k_{n,a}\left[\frac{1}{n}\sqrt{q}n^a M_{jk}\right] + \left[n\sqrt{q}q^{ab}M_{jk}\varphi^k_{,a}\right]_{,b} \\
&\quad + \left[\frac{n}{2}\varphi^k_n\right]\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + 2\left[\frac{n}{2}\varphi^k_n\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] - \left[\frac{n}{2}\Phi_j n^a\right]_{,a}.
\end{aligned} \tag{343}
$$

If we take into account that we can solve for the velocities $\dot{\varphi}^j$ in section 9, then the constraint that arises from $\dot{\Lambda}^{ij}$ will be equal to the constraint c^{jj} in section 9. In case that we can solve for the velocities $\dot{\varphi}^j$ the constraint in $\dot{z}$ reduces to the constraint $-c^{\rm tot}$ with $c^{\rm tot} = c^{\rm geo} + c^{\varphi}$ and c^{φ} includes all fields φ^I, $I = 0, \ldots, 3$, as shown in section 9. For the situation in section 9 $\dot{z}_a$ reduces to $-c^{\rm tot}_a$ plus term proportional to Φ_j which also vanishes there, since in section 9 we have $\Phi_j = 0$ and therefore as displayed in section 9 there would also be no $\dot{\Phi}_j$.

Now we are left with the question how we can make these second class constraints vanish in the context of this section. As we have just discussed choosing $\rho^k = 0$ is necessary to be consistent with the model in section 9. In gravity we have that $\sqrt{q} \neq 0$ and we usually assume $n \neq 0$ and $n^a \neq 0$. Also on the primary constraint surface we have $\Phi_j \approx 0$ and we saw in eq. (334) above that φ^j_n is a Lagrange multiplier. Therefore, we are left with two options making the secondary constraints vanish

(i) $\varphi^j_n = 0$ and $M_{ij} \neq 0$ with $i, j = 1, 2, 3$ for a non-invertible matrix M

(ii) $M_{ij} = 0$ and $\varphi^j_n \neq 0$ with $i, j = 1, 2, 3$ for a non-invertible matrix M

Let us first consider option (i) $\varphi^j_n = 0$ which leads to $\Phi_k = \pi_k$ and we are left with

$$\begin{aligned}
\dot{z} &= -c^{\rm tot,0} - \frac{1}{2}\sqrt{q} M_{ij} q^{ab} \varphi^i_{,a} \varphi^j_{,b}, \qquad (344)\\
\dot{z}_a &= -c^{\rm tot}_a + \frac{1}{2}\varphi^j_{,b}\pi_j + \frac{1}{2}\varphi^j_{,a}\Phi_j,\\
\dot{\Lambda}^{ij} &= -\frac{n}{2}\sqrt{q} q^{ab} \varphi^i_{,a}\varphi^j_{,b},\\
\dot{\Phi}_j &= \nu^b \sqrt{q} M_{jk} \frac{1}{n}\varphi^k_{,b} + \left[\frac{1}{2} n^a \pi_j\right]_{,a} + \left[n\sqrt{q} q^{ab} M_{jk}\varphi^k_{,a}\right]_{,b} - \left[\frac{n}{2}\Phi_j n^a\right]_{,a}.
\end{aligned}$$

On the primary constraint surface for the case $\varphi^j_n = 0$ we have $\Phi_j = \pi_j \approx 0$. Further, we know that the contribution to the diffeomorphism constraint $c^{\rm tot}_a \approx 0$ weakly vanishes on the constraint surface and that the same holds for the contribution to the Hamiltonian constraint $c^{\rm tot,0} + \frac{1}{2}\sqrt{q} M_{ij} q^{ab} \varphi^i_{,a}\varphi^j_{,b} \approx 0$, which leaves us with

$$\dot{\Lambda}^{ij} = -\frac{n}{2}\sqrt{q} q^{ab}\varphi^i_{,a}\varphi^j_{,b}, \qquad (345)$$

$$\dot{\Phi}_j \approx \nu^b \sqrt{q} M_{jk}\frac{1}{n}\varphi^k_{,b} + \left[n\sqrt{q} q^{ab} M_{jk}\varphi^k_{,a}\right]_{,b}. \qquad (346)$$

We already see that the choice $\varphi^j_n = 0$ makes it impossible to compare this model to the one in section 9. To make $\dot{\Lambda}^{ij}$ and $\dot{\Phi}_i$ vanish, we need to choose the Lagrange multiplier $\nu^b = 0$ and $n = 0$. However, the choice $n = 0$ is not consistent with our usual choice $n \neq 0$ in gravity. Moreover, option (i) $\varphi^j_n = 0$ conflicts with our observable construction so far in section 7 and in section 9, since there we have

$$O^{(1)}_{\varphi^j_{,a}}(\sigma) = \delta^j_k, \qquad (347)$$

but for $\varphi^j_n = 0$ we would obtain

$$O^{(1)}_{\dot{\varphi}^j}(\sigma) = O^{(1)}_{n^a\varphi^j_{,a}}(\sigma) = N^j \qquad (348)$$

which is not compatible with our gauge fixing conditions, also compare appendix C.

Next let us consider option (ii) for different numbers of vanishing matrix elements. For a non-invertible matrix M we have a vanishing determinant, i.e. $\det(M) = 0$. Since M is also symmetric, we can bring M into a form where it contains a 2x2 submatrix m and zeros otherwise and we have three independent matrix elements. Now we still have two subcases $\det(m) \neq 0$ and $\det(m) = 0$. For $\det(m) \neq 0$ we can only have two spatial scalar fields which is not suitable for our purpose. However, due to $\det(m) \neq 0$ the submatirx m is invertible and we can solve for the velocities of the two fields, then the constraint Φ_j will not exist. For $\det(m) = 0$ we are only left with one independent degree of freedom, assumed that it does not vanish, it corresponds to one spatial scalar field. Again we can solve for its velocity and Φ_j will not be present but it is not useful for our purpose either. Finally, we assume that a primary constraint $\Phi_j \neq 0$ is present, then all M_{ij} have to be zero but then we have zero spatial scalar fields left and we are again in the situation of [1].

Because we see that the constraint stability analysis in this section contradicts section 7 and also the results we are going to derive in section 9 and is not compatible with our needs to introduce additional reference matter fields, we stop with the constraint stability analysis in this section. Maybe the situation changes if we will not assume M to be a symmetric matrix. However, since we are only interested in finding a quantizable model and this does not bring us any further, we will go on with an even simpler model.

9 Simplest Case Generalization

Large parts of this section have been published in [129] and [130]. Now we assume that the matrix M_{ij} is not only symmetric but even diagonal. This further reduces the additional degrees of freedom, except from the Klein-Gordon fields, from 6 to 3. Note that this is a minimal generalization of the former Klein-Gordon scalar field model in section 7 that can be obtained by choosing $M_{ij} = \delta_{ij}$. Thus, the form of M_{ij} that we work with is

$$\begin{pmatrix} M_{11}(x) & 0 & 0 \\ 0 & M_{22}(x) & 0 \\ 0 & 0 & M_{33}(x) \end{pmatrix}$$

and thus we have three additional degrees of freedom sitting in $M_{jj}(x)$. Because M is diagonal it is also invertible, that is we have $M_{kj}(M^{-1})^{ki} = \delta^i_j = (M^{-1})^{ki} M_{kj}$, where the inverse matrix is defined by $(M^{-1})^{ij} := M^{-1}_{ij}$. Moreover, we even have $i = j$ and for the jth element $M^{-1}_{jj} = \frac{1}{M_{jj}} = (M^{-1})^{jj}$. The form of the action stays the same as for the symmetric matrix and still reads

$$\begin{aligned} S[g, \varphi^0, \varphi^j, M_{ij}] &= \int_M \mathrm{d}^4Y \sqrt{g} R^{(4)} - \frac{1}{2} \int_M \mathrm{d}^4Y \sqrt{g} g^{\mu\nu} \varphi^0_{,\mu} \varphi^0_{,\nu} - \frac{1}{2} \int_M \mathrm{d}^4Y \sqrt{g} M_{ij} g^{\mu\nu} \varphi^i_{,\mu} \varphi^j_{,\nu} \\ &= S^{\mathrm{geo}} + S^{\varphi^0} + S^{\varphi^j}. \end{aligned} \tag{349}$$

9.1 Equations of Motion for the Simplest Generalized Model

We start with the equations of motion that follow from the Euler-Lagrange equation for the variables M_{jj} and obtain for each $j = 1, 2, 3$

$$\frac{\delta S}{\delta M_{jj}} = 0 = -\frac{1}{2} \sqrt{g} g^{\mu\nu} \varphi^j_{,\mu} \varphi^j_{,\nu}. \tag{350}$$

If we define for each $j = 1, 2, 3$ a four velocity $U^\mu_{(j)} := g^{\mu\nu}\varphi^j_{,\nu}$, then the equation above can be rewritten as

$$U^\mu_{(j)}\tilde{\varphi}^j_{,\mu} = \mathcal{L}_{U_{(j)}}\varphi^j = 0, \tag{351}$$

where $\mathcal{L}_{U_{(j)}}$ denotes the Lie derivative with respect to $U^\mu_{(j)}$. Thus, the reference field φ^j is constant along the flow of the vector field $U^\mu_{(j)}$. A similar property can be found in [27], however there the four velocity is not constructed from one scalar field φ^j only but it is constructed from 7 scalar fields T, W_j, S^j where j runs from 1 to 3. Next we discuss the equation of motion for φ^0 which is, as expected, the standard Klein-Gordon equation as can be seen from

$$\begin{aligned} 0 = -\frac{\partial}{\partial x^\mu}\frac{\delta S}{\delta \varphi^0_{,\mu}} &= \partial_\mu\left(\sqrt{g}\varphi^0_{,\nu}g^{\mu\nu}\right) = \sqrt{g}\nabla_\mu\left(g^{\mu\nu}\varphi^0_{,\nu}\right) = \sqrt{g}g^{\mu\nu}\nabla_\mu\varphi^0_{,\nu} = \sqrt{g}\Box^{(g)}\varphi^0 \\ \Longleftrightarrow \quad \Box^{(g)}\varphi^0 = 0, \end{aligned} \tag{352}$$

here ∇_μ defines the torsion free covariant derivative metric compatible with g, compare part II section 1.1, $\Box^{(g)}$ the d'Alembertian operator and we used how covariant derivatives act on tensor densities. Finally, we consider the equations of motion for φ^j. In the former model discussed in section 7 the dynamics of φ^j was also described by a Klein-Gordon equation. This will be modified in the generalized model here. We obtain for each $j = 1, 2, 3$

$$0 = -\frac{\partial}{\partial x^\mu}\frac{\delta S}{\delta \varphi^j_{,\mu}} = \partial_\mu\left(\sqrt{g}M_{jj}\varphi^j_{,\nu}g^{\mu\nu}\right) = \sqrt{g}\nabla_\mu\left(g^{\mu\nu}M_{jj}\varphi^j_{,\nu}\right) = \sqrt{g}g^{\mu\nu}\nabla_\mu(M_{jj}\varphi^j_{,\nu}) \tag{353}$$

as before no summation over repeated j indices is considered here. Hence, the equations of motion for each φ^j are given by

$$M_{jj}\sqrt{g}\Box^{(g)}\varphi^j + \sqrt{g}(\nabla_\mu M_{jj})g^{\mu\nu}\varphi^j_{,\nu} = 0, \tag{354}$$

where again no summation over repeated j indices is assumed. For the reason that the canonical momenta associated with the M_{jj}'s vanish and the M_{jj}'s themselves enter only linearly into the action, the equations of motion do not determine M_{jj} completely. As we will see in the Hamiltonian framework the equations of motion for M_{jj} still include arbitrary Lagrange multipliers. Depending on the choice of these Lagrange multipliers the fields φ^j satisfy the generalized Klein-Gordon equation shown in eq. (354). Comparing with the Brown-Kuchař dust model in [25] the role M_{jj} plays in our model is taken by the scalar fields ρ and W_j in the Brown-Kuchař model. As discussed later, it is exactly this modification for the spatial reference fields that leads to a reduced model whose physical Hamiltonian can be quantized using Loop Quantum Gravity techniques. In section 9.3 we will show that the model is second class and can be reduced to a first class model with only four instead of seven additional scalar fields.

9.2 Total Action in Canonical Form

Since M_{jj} in diagonal form is invertible, we are now able to solve for the velocities of the φ^j fields. Namely, $\pi_j = \sqrt{q}M_{jk}\varphi^k_n = \sqrt{q}\sum_{j=1}^3 M_{jj}\varphi^j_n$ which is equivalent to $\varphi^j_n = \frac{1}{\sqrt{q}}\sum_{j=1}^3(M^{-1})^{jj}\pi_j$ which leads to the velocities

$$\dot{\varphi}^j = \frac{n}{\sqrt{q}}\sum_{j=1}^3(M^{-1})^{jj}\pi_j + n^a\varphi^j_{,a}, \tag{355}$$

here we mean with M_{jj} the elements of the diagonal matrix M and with $(M^{-1})^{jj}$ the elements of its inverse and for the conjugate momentum π_0 to the field φ^0 we still have $\pi_0 = \sqrt{q}\varphi^0_n$, so its velocity is still given by

$$\dot{\varphi}^0 = \frac{n}{\sqrt{q}}\pi_0 + n^a\varphi^j_{,a}. \tag{356}$$

Therefore, we are left with only three primary constraints

$$\begin{aligned} \Lambda^{jj} &:= \Pi^{jj} := \frac{\delta S}{\delta \dot{M}_{jj}} = 0, \\ z &:= p := \frac{\delta S}{\delta \dot{n}} = 0, \\ z_a &:= p_a := \frac{\delta S}{\delta \dot{n}_a} = 0, \end{aligned} \tag{357}$$

here is no summation over the repeated index jj.

Again we perform the Legendre-Transformation which leads to the total action in canonical form

$$\begin{aligned} &S[q_{ab}, p^{ab}, n, p, n^a, p_a, \varphi^0, \pi_0, \varphi^j, \pi_j, M_{jj}, \Pi^{jj}] \\ &= \int_{\mathbb{R}} dt \int_{\chi} \mathrm{d}^3x \left(\frac{1}{\kappa}\dot{q}_{ab}p^{ab} + \dot{\varphi}^0\pi_0 + \sum_{j=1}^{3} \dot{\varphi}^j\pi_j + \dot{n}p + \dot{n}^a p_a + \sum_{j=1}^{3} \dot{M}_{jj}\Pi^{jj} - h_{\text{primary}} \right) \end{aligned} \tag{358}$$

with primary Hamiltonian

$$\begin{aligned} H_{\text{primary}} &= \int_{\chi} \mathrm{d}^3x\, h_{\text{primary}} \\ &= \int_{\chi} d^3x \left(\frac{1}{\kappa}\dot{q}_{ab}p^{ab} - \mathcal{L}_{\text{geo}} + \dot{\varphi}^0\pi_0 + \sum_{j=1}^{3} \dot{\varphi}^j\pi_j - \mathcal{L}_{\varphi} + \nu z + \nu^a z_a + \sum_{j=1}^{3} \mu_{jj}\Lambda^{jj} \right). \end{aligned} \tag{359}$$

Note that here we write down the summation over repeated j-indices explicitly for later convenience.

The terms $\frac{1}{\kappa}p^{ab}q_{ab,t} - \mathcal{L}_{\text{geo}}$ give rise to the geometric part of the Hamiltonian and diffeomorphism constraints c^{geo} and c^{geo}_a already displayed in [26]. From $\dot{\varphi}^0\pi_0 + \sum_{j=1}^{3} \dot{\varphi}^j\pi_j - \mathcal{L}_{\varphi}$ we determine the part of the constraints belonging to the four Klein-Gordon fields which is

$$
\begin{aligned}
&\dot{\varphi}^0\pi_0 + \sum_{j=1}^{3}\dot{\varphi}^j\pi_j - \mathcal{L}_\varphi && (360)\\
&= n\frac{\pi_0^2}{\sqrt{q}} + n^a\,\pi_0\varphi^0_{,a} + n\sum_{j=1}^{3}(M^{-1})^{jj}\,\frac{\pi_j\pi_j}{\sqrt{q}} + n^a\sum_{j=1}^{3}\pi_j\varphi^j_{,a}\\
&- \frac{1}{2}n\sqrt{q}\left(\left[\varphi^0_n\right]^2 - q^{ab}\varphi^0_{,a}\varphi^0_{,b} + \sum_{j=1}^{3}M_{jj}\varphi^j_n\varphi^j_n - \sum_{j=1}^{3}M_{jj}q^{ab}\varphi^j_{,a}\varphi^j_{,b}\right)\\
&= n\frac{1}{2}\sqrt{q}\left(\frac{\pi_0^2}{q} + q^{ab}\varphi^0_{,a}\varphi^0_{,b}\right) + n\frac{1}{2}\sqrt{q}\sum_{j=1}^{3}\left((M^{-1})^{jj}\,\frac{\pi_j\pi_j}{q} + M_{jj}q^{ab}\varphi^j_{,a}\varphi^j_{,b}\right)\\
&+ n^a\left(\pi_0\varphi^0_{,a} + \sum_{j=1}^{3}\pi_j\varphi^j_{,a}\right)\\
&= n\left[\frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} + \sum_{j=1}^{3}\left(\frac{(M^{-1})^{jj}\pi_j\pi_j}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}M_{jj}\varphi^j_{,a}\varphi^j_{,b}\right)\right]\\
&+ n^a\left(\pi_0\varphi^0_{,a} + \sum_{j=1}^{3}\pi_j\varphi^j_{,a}\right)\\
&=: n\,c^\varphi + n^a\,c^\varphi_a .
\end{aligned}
$$

By defining $c^{\text{tot}} := c^{\text{geo}} + c^\varphi$ and $c^{\text{tot}}_a := c^{\text{geo}}_a + c^\varphi_a$ we can write the primary Hamiltonian as

$$
\begin{aligned}
H_{\text{primary}} &= \int_\chi \mathrm{d}^3x\, h_{\text{primary}} && (361)\\
&= \int_\chi \mathrm{d}^3x\left(nc^{\text{tot}} + n^a c^{\text{tot}}_a + \nu z + \nu^a z_a + \sum_{j=1}^{3}\mu_{jj}\Lambda^{jj}\right).
\end{aligned}
$$

Finally, the action in canonical form becomes

$$
\begin{aligned}
&S[q_{ab}, p^{ab}, n, p, n^a, p_a, \varphi^0, \pi_0, \varphi^j, \pi_j, M_{jj}, \Pi^{jj}] && (362)\\
&= \int_{\mathbb{R}} dt\int_\chi \mathrm{d}^3x\left(\frac{1}{\kappa}\dot{q}_{ab}p^{ab} + \dot{\varphi}^0\pi_0 + \sum_{j=1}^{3}\dot{\varphi}^j\pi_j + \dot{n}p + \dot{n}^a p_a + \sum_{j=1}^{3}\dot{M}_{jj}\Pi^{jj} - h_{\text{primary}}\right)
\end{aligned}
$$

with primary constraints

$$z := p, \quad z_a := p_a, \quad \Pi^{ij} := \Lambda^{ij}$$

and we defined that

$$c^{\text{tot}} := c^{\text{geo}} + c^\varphi, \quad c^{\text{tot}}_a := c^{\text{geo}}_a + c^\varphi_a$$

with

$$\kappa c^{\text{geo}} = \frac{1}{\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right)p^{ab}p^{cd} - \sqrt{q}R^{(3)}, \tag{363}$$
$$c^{\varphi} = \frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} + \sum_{j=1}^{3}\left(\frac{(M^{-1})^{jj}\pi_j\pi_j}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}M_{jj}\varphi^j_{,a}\varphi^j_{,b}\right),$$
$$\kappa c^{\text{geo}}_a = -2q_{ac}D_b p^{bc},$$
$$c^{\varphi}_a = \pi_0\varphi^0_{,a} + \sum_{j=1}^{3}\pi_j\varphi^j_{,a}.$$

9.3 Constraint Stability Analysis

In the following we need to perform the constraint analysis in order to check whether the primary constraints are stable under time evolution with respect to H_{primary} or not. The non-vanishing Poisson brackets on the phase space are given by

$$\{q_{cd}(x), p^{ab}(y)\} = \kappa\delta^a_{(c}\delta^b_{d)}\delta^{(3)}(x,y), \tag{364}$$
$$\{n(x), p(y)\} = \delta^{(3)}(x,y),$$
$$\{n^a(x), p_b(y)\} = \delta^a_b\delta^{(3)}(x,y),$$
$$\{\varphi^0(x), \pi_0(y)\} = \delta^{(3)}(x,y),$$
$$\{\varphi^j(x), \pi_k(y)\} = \delta^j_k\delta^{(3)}(x,y),$$
$$\{M_{jj}(x), \Pi^{kk}(y)\} = \delta^k_j\delta^{(3)}(x,y).$$

We need to calculate the Poisson brackets or respectively secondary constrainst

$$\dot{z} = \{z, H_{\text{primary}}\} = \{p, H_{\text{primary}}\}, \tag{365}$$
$$\dot{z}_a = \{z_a, H_{\text{primary}}\} = \{p_a, H_{\text{primary}}\},$$
$$\dot{\Lambda}^{jj} = \{\Lambda^{jj}, H_{\text{primary}}\} = \{\Pi^{jj}, H_{\text{primary}}\}.$$

The details of this calculation can be found in section E of the appendix. In summary the constraint stability analysis of the primary constraints z, z_a and Λ^{jj} leads to

$$\dot{z} = \{z, H_{\text{primary}}\} = \{p, H_{\text{primary}}\} = -c^{\text{tot}}, \tag{366}$$
$$\dot{z}_a = \{z_a, H_{\text{primary}}\} = \{p_a, H_{\text{primary}}\} = -c^{\text{tot}}_a,$$
$$\dot{\Lambda}^{jj} = \{\Lambda^{jj}, H_{\text{primary}}\} = \{\Pi^{jj}, H_{\text{primary}}\} = \frac{n}{2}\left[\frac{(M^{-1})^{jk}(M^{-1})^{j\ell}\pi_k\pi_\ell}{2\sqrt{q}} - \sqrt{q}q^{ab}\varphi^j_{,a}\varphi^j_{,b}\right].$$

9.3.1 Secondary Constraints

In order to ensure that z and z_a are stable we require c^{tot} and c^{tot}_a to be secondary constraints and these are the Hamiltonian and diffeomorphism constraint. We realize that we obtain three more secondary constraints that we denote by c^{jj} which are given by

$$c^{jj} := \frac{n}{2}\left[\frac{(M^{-1})^{jk}(M^{-1})^{j\ell}\pi_k\pi_\ell}{\sqrt{q}} - \sqrt{q}q^{ab}\varphi^j_{,a}\varphi^j_{,b}\right]. \tag{367}$$

We obtained a set of secondary constraints $\{c^{\text{tot}}, c^{\text{tot}}_a, c^{jj}\}$.

9.3.2 Tertiary Constraints

Now given the set of secondary constraints $\{c^{\rm tot}, c_a^{\rm tot}, c^{jj}\}$ we need to compute whether these constraints are stable with respect to $H_{\rm primary}$ or whether tertiary constraints occur. For writing comfort we define $M^{00} := (M^{-1})^{00} := \mathbb{1}_3$ and $I, J = 0,1,2,3$. We display the calculations in some detail here, for even more details see appendix E.

Tertiary Constraint $\dot{c}^{tot}(n)$
We define the smeared constraint $c^{\rm tot}(n) := \int_\chi \mathrm{d}^3x\, n(x) c^{\rm tot}(x)$ and calculate

$$\begin{aligned}
&\{c^{tot}(n), H_{\rm primary}\} \\
&= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm tot}(x), \nu(y)z(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm tot}(x), \nu^b(y)z_b(y)\} \\
&+ \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm tot}(x), \sum_{k=1}^{3} \mu_{kk}(y)\Lambda^{kk}(y)\} \\
&+ \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm tot}(x), n'(y)c^{\rm tot}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm tot}(x), n'^b(y)c_b^{\rm tot}(y)\}.
\end{aligned} \tag{368}$$

For the single terms we obtain the expressions:

1. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm tot}(x), \nu(y)z(y)\} = c^{\rm tot}(\nu)$
2. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm tot}(x), \nu^b(y)z_b(y)\} = 0$
3. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{tot}(x), \mu_{kk}(y)\Pi^{kk}(y)\} = -\int_\chi \mathrm{d}^3x \sum_{j=1}^{3} \mu_{jj}(x)c^{jj}(x) := -c(\mu)$

Since the fourth and the fifth term are rather lengthy, we display them here separately divided again into subterms.

4. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm tot}(x), n'(y)c^{\rm tot}(y)\}$
$= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm geo}(x), n'(y)c^{\rm tot}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\varphi}(x), n'(y)c^{\rm tot}(y)\}$
$= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm geo}(x), n'(y)c^{\rm geo}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm geo}(x), n'(y)c^{\varphi}(y)\}$
$+ \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\varphi}(x), n'(y)c^{\rm geo}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\varphi}(x), n'(y)c^{\varphi}(y)\}$

   4.1. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm geo}(x), n'(y)c^{\rm geo}(y)\} = \{c^{\rm geo}(n), c^{\rm geo}(n')\} = \vec{c}^{\rm geo}\left(q^{-1}\left[n\mathrm{d}n' - n'\mathrm{d}n\right]\right)$

   4.2. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\rm geo}(x), n'(y)c^{\varphi}(y)\}$
   $= -\int_\chi \mathrm{d}^3x\, nn' \frac{1}{\sqrt{q}} c^{\varphi} q_{ab} p^{ab} + \int_\chi \mathrm{d}^3x\, nn' \frac{4}{\sqrt{q}} \left[\sum_{J=0}^{3} \frac{1}{2} M_{JJ} \sqrt{q} \varphi^J_{,e} \varphi^J_{,f}\right] p^{ef}$

   4.3. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n(x)c^{\varphi}(x), n'(y)c^{\rm geo}(y)\}$
   $= \int_\chi \mathrm{d}^3x\, nn' \frac{1}{\sqrt{q}} c^{\varphi} q_{ab} p^{ab} - \int_\chi \mathrm{d}^3x\, nn' \frac{4}{\sqrt{q}} \left[\sum_{J=0}^{3} \frac{1}{2} M_{JJ} \sqrt{q} \varphi^J_{,e} \varphi^J_{f}\right] p^{ef}$

4.4. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^\varphi(x), n'(y)c^\varphi(y)\}$
$= \vec{c}^\varphi \left(q^{-1}\left[n\,\mathrm{d}n' - n'\,\mathrm{d}n\right]\right)$

We see that the terms 4.2. and 4.3. cancel each other so that in the end we are left with

4. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^{\mathrm{tot}}(x), n'(y)c^{\mathrm{tot}}(y)\}$
$= \vec{c}^{\mathrm{geo}} \left(q^{-1}\left[n\,\mathrm{d}\,n' - n'\mathrm{d}n\right]\right) + \vec{c}^\varphi \left(q^{-1}\left[n\,\mathrm{d}n' - n'\,\mathrm{d}n\right]\right) = \vec{c}^{\mathrm{tot}} \left(q^{-1}\left[n\,\mathrm{d}\,n' - n'\mathrm{d}n\right]\right)$

5. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^{\mathrm{tot}}(x), n'^b(y)c^{\mathrm{tot}}_b(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^{\mathrm{geo}}(x), n'^b(y)c^{\mathrm{geo}}_b(y)\} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^{\mathrm{geo}}(x), n'^b(y)c^\varphi_b(y)\}$
$+ \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^\varphi(x), n'^b(y)c^{\mathrm{geo}}_b(y)\} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^\varphi(x), n'^b(y)c^\varphi_b(y)\}$

5.1. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^{\mathrm{geo}}(x), n'^b(y)c^{\mathrm{geo}}_b(y)\} = \{c^{\mathrm{geo}}(n), \vec{c}^{\mathrm{geo}}(\vec{n}')\} = -c^{\mathrm{geo}}(\pounds_{\vec{n}'}n)$

5.2. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^{\mathrm{geo}}(x), n'^b(y)c^\varphi_b(y)\} = 0$

5.3. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^\varphi(x), n'^b(y)c^{\mathrm{geo}}_b(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \, \left[nf\left(\pounds_{\vec{n}'}\frac{1}{\sqrt{q}}\right)_{cd}\right](x) + \int\limits_\chi \mathrm{d}^3x \, [nk_{ab}]\left(\pounds_{\vec{n}'}\sqrt{q}q^{ab}\right)(x)$

5.4. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^\varphi(x), n'^b(y)c^\varphi_b(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \, \frac{n}{\sqrt{q}}\left(\pounds_{\vec{n}'}f\right)(x) + \int\limits_\chi \mathrm{d}^3x \, n\sqrt{q}q^{cd}\left(\pounds_{\vec{n}'}k\right)_{cd}(x)$

Finally, we obtain for term 5.

5. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y \, \{n(x)c^{\mathrm{tot}}(x), n'^b(y)c^{\mathrm{tot}}_b(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \, \left[nf\left(\pounds_{\vec{n}'}\frac{1}{\sqrt{q}}\right)_{cd}\right] + \int\limits_\chi \mathrm{d}^3x \, [nk_{ab}]\left(\pounds_{\vec{n}'}\sqrt{q}q^{ab}\right) + \int\limits_\chi \mathrm{d}^3x \, \frac{n}{\sqrt{q}}\left(\pounds_{\vec{n}'}f\right) + \int\limits_\chi \mathrm{d}^3x \, n\sqrt{q}q^{cd}\left(\pounds_{\vec{n}'}k\right)_{cd}$
$- c^{\mathrm{geo}}(\pounds_{\vec{n}'}n)$
$= \int\limits_\chi \mathrm{d}^3x \, \left[nf\left(\pounds_{\vec{n}'}\frac{1}{\sqrt{q}}\right)_{cd}\right] + \int\limits_\chi \mathrm{d}^3x \, \frac{n}{\sqrt{q}}\left(\pounds_{\vec{n}'}f\right) + \int\limits_\chi \mathrm{d}^3x \, [nk_{ab}]\left(\pounds_{\vec{n}'}\sqrt{q}q^{ab}\right) + \int\limits_\chi \mathrm{d}^3x \, n\sqrt{q}q^{cd}\left(\pounds_{\vec{n}'}k\right)_{cd}$
$- c^{\mathrm{geo}}(\pounds_{\vec{n}'}n)$
$= \int\limits_\chi \mathrm{d}^3x \, n\left(\pounds_{\vec{n}'}\frac{f}{\sqrt{q}}\right) + \int\limits_\chi \mathrm{d}^3x \, n\left(\pounds_{\vec{n}'}\sqrt{q}q^{ab}k_{ab}\right) - c^{\mathrm{geo}}(\pounds_{\vec{n}'}n)$
$= \int\limits_\chi \mathrm{d}^3x \, n\left(n'^b\frac{f}{\sqrt{q}}\right)_{,b} + \int\limits_\chi \mathrm{d}^3x \, n\left(n'^c\sqrt{q}q^{ab}k_{ab}\right)_{,c} - c^{\mathrm{geo}}(\pounds_{\vec{n}'}n)$
$= -\int\limits_\chi \mathrm{d}^3x \, n_{,b}n'^b\frac{f}{\sqrt{q}} - \int\limits_\chi \mathrm{d}^3x \, n_{,c}n'^c\sqrt{q}q^{ab}k_{ab} - c^{\mathrm{geo}}(\pounds_{\vec{n}'}n)$
$= -\int\limits_\chi \mathrm{d}^3x \, \left(\pounds_{\vec{n}'}n\right)\frac{f}{\sqrt{q}} - \int\limits_\chi \mathrm{d}^3x \, \left(\pounds_{\vec{n}'}n\right)\sqrt{q}q^{ab}k_{ab} - c^{\mathrm{geo}}(\pounds_{\vec{n}'}n)$
$= -\int\limits_\chi \mathrm{d}^3x \, \left(\pounds_{\vec{n}'}n\right)\left(\frac{f}{\sqrt{q}} + \sqrt{q}q^{ab}k_{ab}\right) - c^{\mathrm{geo}}(\pounds_{\vec{n}'}n)$
$= -\int\limits_\chi \mathrm{d}^3x \, \left(\pounds_{\vec{n}'}n\right)c^\varphi(x) = -c^\varphi(\pounds_{\vec{n}'}n) - c^{\mathrm{geo}}(\pounds_{\vec{n}'}n) = -c^{\mathrm{tot}}(\pounds_{\vec{n}'}n),$

where we defined

$$f[\pi, M](x) := \frac{1}{2}\sum_{J=0}^{3}(M^{-1})^{JJ}\pi_J\pi_J, \quad k_{ab}[\varphi, M](x) := \frac{1}{2}\sum_{J=0}^{3} M_{JJ}\varphi^J_{,a}\varphi^J_b. \tag{369}$$

Tertiary Constraint $\dot{\vec{c}}^{\text{tot}}(\vec{n})$
Analogous we define the smeared constraint $\vec{c}^{tot}(\vec{n}) := \int_\chi \mathrm{d}^3x\, n^a(x)c^{\text{tot}}_a(x)$ and calculate

$$\begin{aligned}
&\{\vec{c}^{\text{tot}}(\vec{n}), H_{\text{primary}}\} \\
&= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{tot}_a(x), \nu(y)z(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{tot}}_a(x), \nu^b(y)z_b(y)\} \\
&+ \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{tot}}_a(x), \sum_{k=1}^{3}\mu_{kk}(y)\Lambda^{kk}(y)\} \\
&+ \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{tot}}_a(x), n'(y)c^{\text{tot}}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{tot}}_a(x), n'^b(y)c^{\text{tot}}_b(y)\}.
\end{aligned} \tag{370}$$

1. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{tot}}_a(x), \nu(y)z(y)\} = 0$
2. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{tot}}_a(x), \nu^b(y)z_b(y)\} = \int_\chi \mathrm{d}^3x\, \nu^a(x)c^{\text{tot}}_a(x) = \vec{c}^{\text{tot}}(\vec{\nu})$
3. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{tot}}_a(x), \mu_{kk}(y)\Pi^{kk}(y)\} = 0$
4. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{tot}}_a(x), n'(y)c^{\text{tot}}(y)\}$
   $= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{geo}}_a(x), n'(y)c^{\text{tot}}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\varphi}_a(x), n'(y)c^{\text{tot}}(y)\}$
   $= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{geo}}_a(x), n'(y)c^{\text{geo}}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{geo}}_a(x), n'(y)c^{\varphi}(y)\}$
   $+ \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\varphi}_a(x), n'(y)c^{\text{geo}}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\varphi}_a(x), n'(y)c^{\varphi}(y)\}$
   4.1. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{geo}}_a(x), n'(y)c^{\text{geo}}(y)\} = \{\vec{c}^{\text{geo}}(\vec{n}), c^{\text{geo}}(n')\} = c^{\text{geo}}(\pounds_{\vec{n}}n')$
   4.2. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\text{geo}}_a(x), n'(y)c^{\varphi}(y)\}$
   $= -\int_\chi \mathrm{d}^3x\, \left[n'f\left(\pounds_{\vec{n}}\frac{1}{\sqrt{q}}\right)_{cd}\right](x) - \int_\chi \mathrm{d}^3x\, [n'k_{ab}]\left(\pounds_{\vec{n}}\sqrt{q}q^{ab}\right)(x)$
   4.3. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\varphi}_a(x), n'(y)c^{\text{geo}}(y)\} = 0$
   4.4. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y\, \{n^a(x)c^{\varphi}_a(x), n'(y)c^{\varphi}(y)\}$
   $= -\int_\chi \mathrm{d}^3x\, \frac{n'}{\sqrt{q}}\left(\pounds_{\vec{n}}f\right)(x) - \int_\chi \mathrm{d}^3x\, n'\sqrt{q}q^{cd}\left(\pounds_{\vec{n}}k\right)_{cd}(x)$

with f and k_{ab} as given in eq. (369).

5. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\mathrm{tot}}(x), n'^b(y)c_b^{\mathrm{tot}}(y)\}$
$= \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\mathrm{geo}}(x), n'^b(y)c_b^{\mathrm{tot}}(y)\} + \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\mathrm{tot}}(y)\}$
$= \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\mathrm{geo}}(x), n'^b(y)c_b^{\mathrm{geo}}(y)\} + \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\mathrm{geo}}(x), n'^b(y)c_b^{\varphi}(y)\}$
$+ \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\mathrm{geo}}(y)\} + \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\varphi}(y)\}$

5.1. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\mathrm{geo}}(x), n'^b(y)c_b^{\mathrm{geo}}(y)\} = \{\vec{c}^{\mathrm{geo}}(\vec{n}), \vec{c}^{\mathrm{geo}}(\vec{n'})\} = \vec{c}^{\mathrm{geo}}(\pounds_{\vec{n}}\vec{n}')$

5.2. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\mathrm{geo}}(x), n'^b(y)c_b^{\varphi}(y)\} = 0$

5.3. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\mathrm{geo}}(y)\} = 0$

5.4. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\varphi}(y)\} = \int\limits_\chi d^3x \, \left(n^b n'^a_{,b} - n'^b n^a_{,b}\right) c_a^{\varphi} = \vec{c}^{\varphi}(\pounds_{\vec{n}}\vec{n}')$

The addition of 4.3 and 4.4 leads to $c^{\varphi}(\pounds_{\vec{n}}n')$. In summary we obtain for term 4. and 5.

4. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\mathrm{tot}}(x), n'(y)c^{\mathrm{tot}}(y)\} = c^{\varphi}(\pounds_{\vec{n}}n') + c^{\mathrm{geo}}(\pounds_{\vec{n}}n') = c^{\mathrm{tot}}(\pounds_{\vec{n}}n')$.

5. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{n^a(x)c_a^{\mathrm{tot}}(x), n'^b(y)c_b^{\mathrm{tot}}(y)\} = \vec{c}^{\mathrm{geo}}(\pounds_{\vec{n}}\vec{n}') + \vec{c}^{\varphi}(\pounds_{\vec{n}}\vec{n}') = \vec{c}^{\mathrm{tot}}(\pounds_{\vec{n}}\vec{n}')$

Tertiary Constraint $\dot{c}(r)$

Finally, we consider the stability of c^{jj}. Therefore, we also smear c^{jj} that is $c(r) := \int\limits_\chi d^3x \sum\limits_{j=1}^{3} r_{jj}(x)c^{jj}(x)$ and calculate

$$
\begin{aligned}
&\{c(r), H_{\mathrm{primary}}\} \\
&= \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{\sum_{j=1}^{3} r_{jj}(x)c^{jj}(x), \nu(y)z(y)\} + \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{\sum_{j=1}^{3} r_{jj}(x)c^{jj}(x), \nu^b(y)z_b(y)\} \\
&+ \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{\sum_{j=1}^{3} r_{jj}(x)c^{jj}(x), \sum_{k=1}^{3} \mu_{kk}(y)\Lambda^{kk}(y)\} \\
&+ \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{\sum_{j=1}^{3} r_{jj}(x)c^{jj}(x), n'(y)c^{\mathrm{tot}}(y)\} + \int\limits_\chi d^3x \int\limits_\chi d^3y \, \{\sum_{j=1}^{3} r_{jj}(x)c^{jj}(x), n'^b(y)c_b^{\mathrm{tot}}(y)\}.
\end{aligned}
$$

step by step.

1. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{\sum\limits_{j=1}^{3} r_{jj}(x)c^{jj}(x), \nu(y)z(y)\} = \int\limits_\chi d^3x \, \frac{\nu}{n}(x) \sum\limits_{j=1}^{3} r_{jj}(x)c^{jj}(x) := c(\frac{\nu}{n}r)$

2. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{\sum\limits_{j=1}^{3} r_{jj}(x)c^{jj}(x), \nu^b(y)z_b(y)\} = 0$

3. $\int\limits_\chi d^3x \int\limits_\chi d^3y \, \{\sum\limits_{j=1}^{3} r_{jj}(x)c^{jj}(x), \sum\limits_{k=1}^{3} \mu_{kk}(y)\Lambda^{kk}(y)\}$
$= -\sum\limits_{j=1}^{3} r_{jj}(x)\mu_{jj}(x) \left[n \frac{\left((M^{-1})^{jj}\right)^3 \pi_j \pi_j}{\sqrt{q}} \right](x)$

The terms 4. and 5. need not to be calculated explicitly as we will explain in the subsequent. Here we just notice that they are non-vanishing, i.e.

4. $\int_\chi d^3x \int_\chi d^3y \sum_{j=1}^{3} r_{jj}(x)c^{jj}(x), n'(y)c^{\text{tot}}(y)\} \neq 0$

5. $\int_\chi d^3x \int_\chi d^3y \{\sum_{j=1}^{3} r_{jj}(x)c^{jj}(x), n'^b(y)c_b^{\text{tot}}(y)\} \neq 0$

When computing the stability in the case of c_a^{tot} all non-vanishing contributions are proportional to either c^{tot} or c_a^{tot}. Thus, we can conclude

$$\{c_a^{\text{tot}}, H_{\text{primary}}\} \approx 0. \tag{371}$$

Further, for c^{tot} we have a similar situation. There all non-vanishing contributions are proportional to $c^{\text{tot}}, c_a^{\text{tot}}$ or c^{jj} respectively. Hence, also here we have

$$\{c^{\text{tot}}, H_{\text{primary}}\} \approx 0. \tag{372}$$

For c^{jj} let us consider the individual contributions of the primary Hamiltonian separately. We have

$$\int_\chi d^3y\{c^{jj}(x), (\mu_{kk}\Lambda^{kk})(y)\} = -\mu_{jj}\frac{n}{\sqrt{q}}\pi_j^2((M^{-1})^{jj})^3, \tag{373}$$

again no summation of j is assumed here. The non-vanishing contributions that are not again proportional to already existing constraints come from

$$\int_\chi d^3y\{c^{jj}(x), (nc^{\text{tot}})(y)\} \neq 0 \tag{374}$$

and

$$\int_\chi d^3y\{c^{jj}(x), (n^a c_a^{\text{tot}})(y)\} \neq 0. \tag{375}$$

However, we do not need to compute these contributions in explicit form because the result in eq. (373) involves the Lagrange multipliers μ_{jj} in linear form. Therefore, although we have non-vanishing contributions from the Poisson brackets also on the constraint hypersurface we can solve $\{c^{11}, H_{\text{primary}}\} = 0$ for the Lagrange multiplier μ_{11} and likewise in the cases $j = 2, 3$ where we can solve the corresponding equations for μ_{22} and μ_{33} respectively. As a consequence, the stability is also ensured for c^{jj} and thus the model contains no tertiary constraints and the constraint algorithm stops here. The final set of constraints is given by $\{z, z_a, c_a^{\text{tot}}, c^{\text{tot}}, \Lambda^{jj}, c^{jj}\}$. Now we need to classify the constraints into first and second class. We define the following linear combination of constraints

$$\widetilde{c}_a^{\text{tot}} := c_a^{\text{tot}} + \sum_{j=1}^{3} M_{jj,a}\Pi^{jj} + n_{,a}p + (\pounds_{\vec{n}}p)_a = c_a^{\text{tot}} + \sum_{j=1}^{3} M_{jj,a}\Lambda^{jj} + n_{,a}z + (\pounds_{\vec{n}}z)_a \,. \tag{376}$$

The constraints $\widetilde{c}_a^{\mathrm{tot}}$ are the generator of spatial diffeomorphisms on the phase space with elementary variables $(q_{ab}, p^{ab}, n, p, n^a, p_a, M_{jj}, \Pi^{jj})$ and thus the constraints $\widetilde{c}_a^{\mathrm{tot}}$ are first class constraints. For the constraint c^{tot} we consider the following linear combination

$$\widetilde{c}^{\mathrm{tot}} := c^{\mathrm{tot}} + \sum_{j=1}^{3} \beta_{jj} \Lambda^{jj} \tag{377}$$

and determine β_{jj} such that $\widetilde{c}^{\mathrm{tot}}$ and c^{jj} have vanishing Poisson brackets up to terms proportional to the constraints for all $j = 1, 2, 3$. We have

$$\{\widetilde{c}^{\mathrm{tot}}(x), c^{jj}(y)\} = \{c^{\mathrm{tot}}(x), c^{jj}(y)\} + \beta_{jj} \frac{n}{\sqrt{q}} \frac{\pi_j^2}{(M_{jj})^3} \stackrel{!}{=} 0. \tag{378}$$

9.3.3 Calculation of β_{jj}

Solving this equation for β_{jj} yields

$$\begin{aligned}
\beta_{jj}(x) &= -\int_\chi \mathrm{d}^3y \sqrt{q} \frac{(M_{jj})^3}{n\pi_j^2} \{c^{\mathrm{tot}}(x), c^{jj}(y)\} \\
&= -\int_\chi \mathrm{d}^3y \sqrt{q} \frac{(M_{jj})^3}{n\pi_j^2} \left(\{c^{\mathrm{geo}}(x), c^{jj}(y)\} + \{c^{\phi}(x), c^{jj}(y)\}\right) \\
&= -\sqrt{q} \frac{(M_{jj})^3}{n\pi_j^2} \left(-\frac{1}{2\sqrt{q}} c^{jj} \left(p^{ab} q_{ab}\right) - n\varphi^j_{,a}\varphi^j_{,b}\, p^{ab} \right. \\
&\quad \left. - \left[\frac{(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right] \left[n\sqrt{q} q^{ab} \varphi^j_{,b}\right]_{,a} - \left[\sqrt{q} M_{jj} q^{ab} \varphi^j_{,b}\right]_{,a} \left[n \frac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right]\right) \\
&= \frac{(M_{jj})^3}{2n\pi_j^2} c^{jj} \left(p^{ab} q_{ab}\right) + \sqrt{q} \frac{(M_{jj})^3}{\pi_j^2} \varphi^j_{,a}\varphi^j_{,b}\, p^{ab} + \frac{(M_{jj})^2}{n\pi_j} \left[n\sqrt{q} q^{ab} \varphi^j_{,b}\right]_{,a} + \frac{M_{jj}}{\pi_j} \left[\sqrt{q} M_{jj} q^{ab} \varphi^j_{,b}\right]_{,a},
\end{aligned} \tag{379}$$

where we used the following results of the calculation of the Poisson bracktes.

1. $\int_\chi d^3y \{\kappa c^{\mathrm{geo}}(x), c^{jj}(y)\} = -\kappa \frac{1}{2\sqrt{q}} c^{jj} \left(p^{ab} q_{ab}\right) - \kappa n \varphi^j_{,a}\varphi^j_{,b}\, p^{ab}$
2. $\int_\chi d^3y \{c^{\varphi}(x), c^{jj}(y)\} = -\left[\frac{(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right] \left[n\sqrt{q} q^{ab} \varphi^j_{,b}\right]_{,a} - \left[\sqrt{q} M_{jj} q^{ab} \varphi^j_{,b}\right]_{,a} \left[n \frac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right]$

The rather lengthy but straightforward calculation also presented in more detail in appendix F shows that

$$\begin{aligned}
\beta_{jj}(x) =& \frac{1}{2} \frac{(M_{jj})^3}{n\pi_j^2} q_{ab} p^{ab} c^{jj}(x) + \sqrt{q} \varphi^j_{,a}\varphi^j_{,b} p^{ab} \frac{(M_{jj})^3}{\pi_j^2}(x) \\
&+ \frac{(M_{jj})^2}{n\pi_j} \left(n\sqrt{q} q^{ab} \varphi^j_{,b}\right)_{,a}(x) + \frac{(M_{jj})}{\pi_j} \left(M_{jj}\sqrt{q} q^{ab} \varphi^j_{,b}\right)_{,a}(x).
\end{aligned} \tag{380}$$

On the constraint surface $c^{jj} = 0$ the expression for β_{jj} reduces to

$$\beta_{jj}(x) \approx +\sqrt{q} \varphi^j_{,a}\varphi^j_{,b} p^{ab} \frac{(M_{jj})^3}{\pi_j^2}(x) + \frac{(M_{jj})^2}{n\pi_j} \left(n\sqrt{q} q^{ab} \varphi^j_{,b}\right)_{,a}(x) + \frac{(M_{jj})}{\pi_j} \left(M_{jj}\sqrt{q} q^{ab} \varphi^j_{,b}\right)_{,a}(x). \tag{381}$$

Given this choice of β_{jj} also $\widetilde{c}^{\text{tot}}$ is a first class constraint. The remaining constraints Λ^{jj} and c^{jj} build three second class pairs (c^{11}, Λ_{11}), (c^{22}, Λ_{22}) and (c^{33}, Λ_{33}). Let us shortly summarize. We have extended the four Klein-Gordon scalar fields model by 6 additional degrees of freedom (M_{jj}, Π^{jj}). The constraint analysis showed that our model has four first class constraints $\widetilde{c}_a^{\text{tot}}$ and $\widetilde{c}^{\text{tot}}$ and a system of six second class constraints c^{jj}, Λ^{jj}. Therefore, if we reduce with respect to the second class constraints and consider this partially reduced phase space, we also reduce exactly the six additional degrees of freedom because each second class constraint reduces one degree of freedom in phase space. This partially reduced model consists of gravity plus for scalar fields that we will use as reference fields later in order to derive the reduced phase space with respect to $\widetilde{c}^{\text{tot}}$ and $\widetilde{c}_a^{\text{tot}}$. To perform the reduction with respect to the second class constraints we need to compute the associated Dirac bracket. For this purpose we define the following set of constraints c_I with $I = 1, \cdots, 6$ and $\{c_I\}_{I=1,\cdots,6} = \{c^{jj}, \Lambda^{jj} | j = 1, 2, 3\}$ and introduce the matrix

$$\mathcal{N}_{JK}(x,y) := \{c_J(x), c_K(y)\} = \begin{pmatrix} A_{jk}(x,y) & B_{jk}(x,y) \\ C_{jk}(x,y) & 0 \end{pmatrix} \tag{382}$$

where $A_{jk}(x,y) = \{c^{jj}(x), c^{kk}(y)\}$, $B_{jk}(x,y) = \{c^{jj}(x), \Lambda^{kk}(y)\}$, $C_{jk}(x,y) = \{\Lambda^{jj}(x), c^{kk}(y)\}$ and we used that $\{\Lambda^{jj}(x), \Lambda^{kk}(y)\} = 0$. We have, compare eq. (373),

$$\{c^{jj}(x), \Lambda^{kk}(y)\} = -\frac{n}{\sqrt{q}} \frac{\pi_j^2}{(M_{jj})^3} \delta^{kj} \delta^{(3)}(x,y).$$

and $\{c^{jj}(x), c^{kk}(y)\} = 0$ for $j \neq k$ and as a consequence all 3×3-matrices A, B, C are diagonal matrices. The inverse matrix $(\mathcal{N}^{-1})^{IJ}$ is given by

$$(\mathcal{N}^{-1})^{JK}(x,y) = \begin{pmatrix} 0 & (C^{-1})^{jk}(x,y) \\ (B^{-1})^{jk}(x,y) & -(B^{-1}AC^{-1})^{jk}(x,y) \end{pmatrix} \tag{383}$$

The associated inverse matrix satisfies

$$\int_\chi d^3z \, \mathcal{N}_{IL}(x,z)(\mathcal{N}^{-1})^{LJ}(z,y) = \delta^{(3)}(x,y)\delta_I^J.$$

Given the inverse matrix, we can write down the Dirac bracket that is given by

$$\begin{aligned} \{f,g\}^* &= \{f,g\} - \int_\chi d^3y \int_\chi d^3x \left(\{f, c_J(x)\}(\mathcal{N}^{-1})^{JK}(x,y)\{c_K(y), g\}\right) \\ &= \{f,g\} - \int_\chi d^3y \int_\chi d^3x \left((\{f, c^{jj}(x)\}(C^{-1})^{jk}(x,y)\{\Lambda^{kk}(y), g\}\right. \\ &- \int_\chi d^3y \int_\chi d^3x \{f, \Lambda^{jj}(x)\}(B^{-1})^{jk}(x,y)\{c^{kk}(y), g\} \\ &+ \int_\chi d^3y \int_\chi d^3x \, \{f, \Lambda^{jj}(x)\}(B^{-1}AC^{-1})^{jk}(x,y)\{\Lambda^{kk}(y), g\})). \end{aligned} \tag{384}$$

For the reason that the constraints $\Lambda^{jj} = \Pi^{jj}$ are equal to the canonical momenta of M_{jj} we can immediately conclude that the Dirac bracket for the subset of variables $q_{ab}, p^{ab}, \varphi^0, \pi_0, \varphi^j, \pi_j$

coincides with the usual Poisson bracket because each of the variables commutes with Λ^{jj}. Hence, the Dirac brackets affects the variables (M_{jj}, Π^{jj}) only. The algebra for this subset has the form

$$\{M_{jj}(x), M_{kk}(y)\}^* = -(B^{-1}AC^{-1})^{jk}(x,y), \quad \{\Pi^{jj}(x), \Pi^{kk}(y)\}^* = 0, \quad \{M_{jj}(x), \Pi^{kk}(y)\}^* = 0.$$

To obtain the partially reduced phase space we can set $\Lambda^{jj} = \Pi^{jj} = 0$ and express M_{jj} in terms of the remaining variables using $c^{jj} = 0$. We obtain, compare eq. (367),

$$M_{jj}\Big|_{c^{jj}=0} = \frac{\pi_j}{\sqrt{q}} \frac{1}{\sqrt{q^{ab}\varphi^j_{,a}\varphi^j_{,b}}} \quad \text{for} \quad j = 1,2,3 \tag{385}$$

and as usual no summation over repeated j's is considered here. On this partially reduced phase space the constraint $\widetilde{c}^{\text{tot}}_a$ has the following form

$$\widetilde{c}^{\text{tot}}_a = c^{\text{tot}}_a + n_{,a}z + (\mathcal{L}_{\vec{n}}z)_a.$$

In order to rewrite the constraint $\widetilde{c}^{\text{tot}}$ on the partially reduced phase space we use M_{jj} in eq. (385) leading to

$$\begin{aligned}
\widetilde{c}^{\text{tot}}\Big|_{c^{jj}=0,\Lambda^{jj}=0} &= c^{\text{geo}} + \frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} + \sum_{j=1}^{3} \sqrt{q}M_{jj}q^{ab}\varphi^j_{,a}\varphi^j_{,b} \\
&= c^{\text{geo}} + \frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} + \sum_{j=1}^{3} \pi_j\sqrt{q^{ab}\varphi^j_{,a}\varphi^j_{,b}} \\
&\approx c^{\text{geo}} + \frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} - \sum_{j=1}^{3} \varphi^a_j(c^{\text{geo}}_a + \pi_0\varphi^0_{,a})\sqrt{q^{bc}\varphi^j_{,b}\varphi^j_{,c}}.
\end{aligned} \tag{386}$$

Now as usual in the context of the ADM formalism we go to the reduced ADM phase space, that is the one where a reduction with respect to the primary constraints z and z_a has been performed. In the reduced ADM phase space we can treat the lapse function n and the shift vector n^a as Lagrange multipliers. On the reduced ADM phase space we have $\widetilde{c}^{\text{tot}}_a = c^{\text{tot}}_a$. Summarizing, starting from the model whose action is given in eq. (349), we end up with a reduced ADM phase space with elementary variables $(q_{ab}, p^{ab}, \varphi^J, \pi_J)$, for $J = 0, \ldots, 3$, which is a model consisting of gravity and four scalar fields and a set of first class constraints given by

$$\begin{aligned}
c^{\text{tot}}_a &= c^{\text{geo}}_a + \pi_0\varphi^0_{,a} + \pi_j\varphi^j_{,a}, \\
c^{\text{tot}} &= c^{\text{geo}} + \frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} - \sum_{j=1}^{3} \varphi^a_j(c^{\text{geo}}_a + \pi_0\varphi^0_{,a})\sqrt{q^{bc}\varphi^j_{,b}\varphi^j_{,c}}.
\end{aligned} \tag{387}$$

In the next subsection we will discuss the construction of observables for this model.

9.4 Step 1: Construction of Observables

Here we will follow very closely the presentation in section 7.3 because most of the steps performed for the four Klein-Gordon scalar fields model carry over to the generalized model. Again we start by rewriting the constraint in Abelianized form.

9.4.1 Weakly Abelian Set of Constraints

For this purpose we start with c^{tot} in eq. (387) and solve it ($c^{\mathrm{tot}} = 0$) for the reference field momentum π_0. We get

$$\pi_0^2 - \pi_0 \left(2\sqrt{q} \sum_{j=1}^{3} \varphi^0_{,a} \varphi^a_j \sqrt{q^{cd} \varphi^j_{,c} \varphi^j_{,d}} \right) + q q^{ab} \varphi^0_{,a} \varphi^0_{,b} - 2\sqrt{q} \sum_{j=1}^{3} \varphi^a_j c^{\mathrm{geo}}_a \sqrt{q^{bc} \varphi^j_{,b} \varphi^j_{,c}} + 2\sqrt{q} c^{\mathrm{geo}} = 0. \tag{388}$$

We define the following abbreviations:

$$\begin{aligned} b &:= -2\sqrt{q} \sum_{j=1}^{3} \varphi^0_{,a} \varphi^a_j \sqrt{q^{cd} \varphi^j_{,c} \varphi^j_{,d}}, \\ c &:= q q^{ab} \varphi^0_{,a} \varphi^0_{,b} - 2\sqrt{q} \sum_{j=1}^{3} \varphi^a_j c^{\mathrm{geo}}_a \sqrt{q^{bc} \varphi^j_{,b} \varphi^j_{,c}} + 2\sqrt{q} c^{\mathrm{geo}}, \end{aligned} \tag{389}$$

then solving for the momentum π_0 yields

$$\pi_0 = -\frac{b}{2} \pm \sqrt{\left(\frac{b}{2}\right)^2 - c} =: -h(q_{ab}, p^{ab}, \varphi^0, \varphi^j) =: -h. \tag{390}$$

As before, in order to ensure that the final physical Hamiltonian is positive, we choose the plus sign for the square root here in order to define h. The spatial diffeomorphism constraint c^{tot}_a can as in the former model be solved for π_j using the inverse φ^a_j of $\varphi^j_{,a}$ leading to

$$\pi_j = -\varphi^a_j \left(c^{\mathrm{geo}}_a + \pi_0 \varphi^0_{,a} \right) =: -h_j(q_{ab}, p^{ab}, \varphi^j, \varphi^0) := -h_j. \tag{391}$$

Likewise to the model discussed in section 7 we can write down the following Abelian set of equivalent constraints

$$\begin{aligned} c^{\mathrm{tot}} &:= \pi_0 + h(q_{ab}, p^{ab}, \varphi^0, \varphi^j), \\ c^{\mathrm{tot}}_j &:= \pi_j + h_j(q_{ab}, p^{ab}, \varphi^0, \varphi^j), \end{aligned} \tag{392}$$

where h and h_j are the functions defined in eq. (390) and eq. (391). We consider this set of Abelian first class constraints in the section where observables with respect to these constraints are constructed.

9.4.2 Explicit Construction of the Observables

We can apply the observable map as was presented in section 5 and carried out for the four standard Klein-Gordon fields in section 7. Hence, we will first construct observables with respect to the spatial diffeomorphism constraint c^{tot}_j and afterwards with respect to the Hamiltonian constraint c^{tot}. Since we have explained the individual steps of the construction in section 7.3 and these can be carried over to the generalized model here, we will just present the results here. As before for all but the reference fields φ^j we construct the following quantities:

$$\varphi^0, \quad \pi_0/J, \quad q_{jk} = q_{ab} \varphi^a_j \varphi^b_k, \quad p^{jk} = p^{ab} \varphi^j_{,a} \varphi^k_{,b}/J, \tag{393}$$

where $J := |\det(\varphi^j/\partial_x)|$ is, as before, used to transform scalar/tensor densities into real scalars/tensors. Then the observables with respect to c_j^{tot} are given by

$$\widetilde{\varphi}^0 := O^{(1)}_{\varphi^0,\{\varphi^j\}}(\sigma) = \int\limits_\chi d^3x \big|\det(\partial\varphi^j/\partial_x)\big|\delta(\varphi^j(x),\sigma^j)\varphi^0(x), \tag{394}$$
$$\widetilde{\pi}_0 := O^{(1)}_{\pi_0,\{\varphi^j\}}(\sigma) = \int\limits_\chi d^3x\, \delta(\varphi^j(x),\sigma^j)\pi_0(x),$$
$$\widetilde{q}_{jk} := O^{(1)}_{q_{ab},\{\varphi^j\}}(\sigma) = \int\limits_\chi d^3x \big|\det(\partial\varphi^j/\partial_x)\big|\delta(\varphi^j(x),\sigma^j)\varphi^a_j\varphi^b_k q_{ab}(x),$$
$$\widetilde{p}^{jk} := O^{(1)}_{p^{ab},\{\varphi^j\}}(\sigma) = \int\limits_\chi d^3x\, \delta(\varphi^j(x),\sigma^j)\varphi^j_a\varphi^k_b p^{ab}.$$

Here we used the integral representation for the observables introduced in section 7. For the reference fields the observable map leads to:

$$\widetilde{\varphi}^j = O^{(1)}_{\varphi^j,\{\varphi^j\}}(\sigma) = \Big[\alpha^{K_{\beta_1}}_{\beta_1}(\varphi^j)\Big]_{\alpha_t^{K_{\beta_1}}(\varphi^j)=\sigma^j} = \sigma^j, \tag{395}$$
$$\widetilde{\pi}_j = O^{(1)}_{\pi_j,\{\varphi^j\}}(\sigma) = \int\limits_\chi d^3x \big|\det(\partial\varphi^j/\partial_x)\big|\delta(\varphi^j(x),\sigma^j)\pi_j(x).$$

The spatially diffeomorphism invariant observables of the constraints are given by

$$\widetilde{c}^{\text{tot}} = \widetilde{\pi}_0 + \widetilde{h}, \tag{396}$$
$$\widetilde{c}_j^{\text{tot}} = \widetilde{\pi}_j + \widetilde{c}_j^{\text{geo}} - \widetilde{h}\widetilde{\varphi}^0_{,j} = \widetilde{\pi}_j + \widetilde{c}_j^{\text{geo}} - \widetilde{h}\widetilde{\varphi}^0_{,j},$$

where we used that

$$O^{(1)}_{\varphi^j_{,a}}(\sigma) = \int\limits_\chi d^3x \big|\det(\partial\varphi^j/\partial_x)\big|\delta(\varphi^j(x),\sigma^j)\varphi^j_{,a}\varphi^a_k = \delta^j_k \tag{397}$$

and likewise $O^{(1)}_{\varphi^a_{,j}}(\sigma) = \delta^k_j$. The observables with respect to the diffeomorphism constraint associated with h denoted as $\widetilde{h}$ can be easily obtained by using the property of the observable map. This implies that $\widetilde{h} = h(\widetilde{q}_{jk}, \widetilde{p}^{jk}, \widetilde{\varphi}^j, \widetilde{\varphi}^j)$. Using this we obtain

$$\widetilde{h} = -\sqrt{\widetilde{q}}\widetilde{\varphi}^0_{,j}\sqrt{\widetilde{q}^{jk}\delta_{jk}} + \sqrt{\left(\sqrt{\widetilde{q}}\widetilde{\varphi}^0_{,j}\sqrt{\widetilde{q}^{jk}\delta_{jk}}\right)^2 - \widetilde{q}\widetilde{q}^{jk}\widetilde{\varphi}^0_{,j}\widetilde{\varphi}^0_{,k} + 2\sqrt{\widetilde{q}}\sum_{j=1}^{3}\widetilde{c}_j^{\text{geo}}\sqrt{\widetilde{q}^{jj}} - 2\sqrt{\widetilde{q}}\widetilde{c}^{\text{geo}}} \tag{398}$$
$$= -\sqrt{\widetilde{q}}\widetilde{\varphi}^0_{,j}\sqrt{\widetilde{q}^{jk}\delta_{jk}} + \sqrt{\left(\sqrt{\widetilde{q}}\widetilde{\varphi}^0_{,j}\sqrt{\widetilde{q}^{jk}\delta_{jk}}\right)^2 - \widetilde{q}\widetilde{q}^{jk}\widetilde{\varphi}^0_{,j}\widetilde{\varphi}^0_{,k} + 2\sqrt{\widetilde{q}}\sum_{j=1}^{3}\sqrt{\widetilde{q}^{jj}\widetilde{c}_j^{\text{geo}}\widetilde{c}_j^{\text{geo}}} - 2\sqrt{\widetilde{q}}\widetilde{c}^{\text{geo}}}.$$

Next we want to derive the observables with respect to $\widetilde{c}^{\text{tot}}$ and also here we can exactly follow the construction discussed in section 7.3. For this generalized model the full observables that we as before denote with capital letters are given by

$$
\begin{aligned}
Q_{jk}(\sigma,\tau) &:= O_{q_{ab},\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{q}_{jk}(\sigma),\widetilde{\varphi}^0}, \\
P^{jk}(\sigma,\tau) &:= O_{p^{ab},\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{p}^{jk}(\sigma),\widetilde{\varphi}^0}, \\
\Pi_0(\sigma,\tau) &:= O_{\pi_0,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{\pi}_0(\sigma),\widetilde{\varphi}^0}, \\
\Pi_j(\sigma,\tau) &:= O_{\pi_j,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = O^{(2)}_{\widetilde{\pi}_j(\sigma),\widetilde{\varphi}^0}.
\end{aligned}
\tag{399}
$$

Note that also here Π_0 and Π_j are no independent observables for the reason that these can be expressed in terms of Q^{jk} and P_{jk} using the constraints in eq. (392). Furthermore for the four reference fields we have

$$
O_{\varphi^0,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = \tau \quad \text{and} \quad O_{\varphi^j,\{\varphi^0,\varphi^j\}}(\sigma,\tau) = \sigma^j. \tag{400}
$$

Hence, the elementary variables of the reduced phase space are (Q_{jk}, P^{jk}). This finishes our discussion on the full observables and in the next section we are going to derive the physical Hamiltonian that is generating their dynamics on the reduced phase space.

9.5 Step 2: Dynamics encoded in the Physical Hamiltonian

We have already shown in section 7.3 that even if the constraints do not deparametrize the physical Hamiltonian density is given by the full observables associated with the phase space function h that occurs in the rewritten version of the Hamiltonian constraint in eq. (392). The same applies to the generalized model considered here. Using that the physical Hamiltonian is as before given by

$$
\mathbf{H}_{\text{phys}} := \int\limits_{\mathcal{S}} d^3\sigma O^{(2)}_{\widetilde{h}(\sigma),\widetilde{\varphi}^0}(\sigma,\tau) = \int\limits_{\mathcal{S}} d^3\sigma H(\sigma,\tau), \tag{401}
$$

here we denote the (full) observable associated to h according to our notation by H. Now looking into eq. (398) and using the property of the observable map we get for the physical Hamiltonian density

$$
H(\sigma) = \sqrt{-2\sqrt{Q}C^{\text{geo}} + 2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C^{\text{geo}}_jC^{\text{geo}}_j}(\sigma)}. \tag{402}
$$

We realize that the final physical Hamiltonian density is independent of the physical time τ because the reference field $\widetilde{\varphi}^0$ occurred only via spatial derivatives and as pointed out already in [23] and also discussed in 7.3, we have $O^{(2)}_{\widetilde{\varphi}^0_{,j},\widetilde{\varphi}^0}(\sigma,\tau) = d\tau/d\sigma^j = 0$. Therefore, all terms that involve $\widetilde{\varphi}^0_{,j}$ in $\widetilde{h}$ in eq. (398) will be vanishing at the observable level. Let us compare the form of the physical Hamiltonian density in the four scalar field model shown in eq. (320). First let us check that the density weight is correct in both cases. Each of the terms under the square root has density weight two and hence the physical Hamiltonian density is of weight one as it should be. The same is true for the physical Hamiltonian density in eq. (402) of our generalized model. The main difference between the two models is that the term $\delta^{jk}C^{\text{geo}}_jC^{\text{geo}}_k$ that occurred in eq. (320) and that prohibited the completion of the reduced quantization program in the case of the four Klein-Gordon scalar fields model, is no longer present in eq. (402). Instead the physical Hamiltonian density for the generalized model contains terms of the form $Q^{jj}C^{\text{geo}}_jC^{\text{geo}}_j$ for $j = 1, 2, 3$. As we will discuss in the next subsection, it is exactly this feature of the model that allows to complete the reduced quantization program.

9.6 Step 3: Reduced Quantization

Given the fact that we want to quantize the reduced theory using techniques from Loop Quantum Gravity, we will reformulate the reduced phase space in terms of Ashtekar variables (A^A_j, E^j_A). Also in the generalized model the observable algebra of the elementary variables (A^A_j, E^j_A) is isomorphic to the kinematical subalgebra of (A^j_a, E^a_j) and as discussed in detail in section 7.5 because of this we can use the usual Ashtekar-Lewandowski representation of Loop Quantum Gravity to obtain the physical Hilbert space $\mathcal{H}_{phys}$ of the generalized model. As before the price to pay when working in the connection formulation instead of the ADM formulation is an additional SU(2) Gauss constraint. However, this can simply be solved in the quantum theory by restricting to only gauge invariant spin networks in $\mathcal{H}_{phys}$. Where the quantization program stopped in the four Klein-Gordon scalar field case, when we wanted to implement the physical Hamiltonian $\mathbf{H}_{\text{phys}}$ as an operator on $\mathcal{H}_{phys}$, now the situation has changed. The individual terms that occur under the square root of the physical Hamiltonian density in eq. (402) can all be quantized on $\mathcal{H}_{phys}$ using Loop Quantum Gravity techniques. Let us consider the first term, that is $-2\sqrt{Q}C^{\text{geo}}$. The two individual contributions of $\sqrt{Q}$ and C^{geo} will be quantized as individual operators. The first one, $\sqrt{Q}$ can be quantized by means of the volume operator [114, 116]. The observable associated to the geometric part of the Hamiltonian constraint C^{geo} can be quantized using the techniques introduced in [138]. For the quantization of the second term $2\sqrt{Q}\sum\limits_{j=1}^{3}\sqrt{Q^{jj}C^{\text{geo}}_j C^{\text{geo}}_j}$, we will promote the entire term to an operator at the quantum level and this can be done using the usual quantization for holonomies and fluxes in Loop Quantum Gravity. Note that the quantization used in [5] for the Brown-Kuchař dust model does not carry over to this model because here the second term does not involve a covariant contraction of the spatial indices between the observables associated with the metric Q^{jk} and the geometric part of the spatial diffeomorphism constraint C^{geo}_j. As a consequence, a different regularization procedure needs to be considered.

We start from the classical expression of the physical Hamiltonian given by:

$$\mathbf{H}_{\text{phys}} = \int\limits_{\mathcal{S}} d^3\sigma \sqrt{-2\sqrt{Q}C^{\text{geo}} + 2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C^{\text{geo}}_j C^{\text{geo}}_j}}(\sigma). \tag{403}$$

Likewise to the volume operator or the physical Hamiltonian in [1, 3] the classical expression involves a square root. From the classical point of view, the physical Hamiltonian density is real and this is only true if $-2\sqrt{Q}C^{\text{geo}} + 2\sqrt{Q}\sum\limits_{j=1}^{3}\sqrt{Q^{jj}C^{\text{geo}}_j C^{\text{geo}}_j} \geq 0$. In deriving the form of $\mathbf{H}_{\text{phys}}$ we restrict to the part of the phase space in which $C^{\text{geo}} \leq 0$. Moreover, from the classical Hamiltonian constraint equation we get

$$\pi_0^2 - \pi_0\left(2\sqrt{q}\sum_{j=1}^{3}\varphi^0_{,a}\varphi^a_j\sqrt{q^{cd}\varphi^j_{,c}\varphi^j_{,d}}\right) + qq^{ab}\varphi^0_{,a}\varphi^0_{,b} - 2\sqrt{q}\sum_{j=1}^{3}\varphi^a_j c^{\text{geo}}_a\sqrt{q^{bc}\varphi^j_{,b}\varphi^j_{,c}} + 2\sqrt{q}c^{\text{geo}} = 0.$$

Applying the observable map to the equation above yields

$$\Pi_0^2 = H^2(\sigma), \tag{404}$$

where Π_0 denotes the observable associated with π_0 and $H^2(\sigma)$ is the square of the physical Hamiltonian density $H(\sigma)$, that is the expression under the square root in eq. (403). Note that we applied the observable map with $J := |\det(\partial\varphi^j/\partial_x)| > 0$. Considering eq. (404) we realize that on the physical part of the phase space we have that $H^2(\sigma)$ is non-negative due to the reason that certainly $\Pi_0^2 \geq 0$. However, this does not ensure that the quantized version of $H^2(\sigma)$ is non-negative. In principle, we can achieve this by implementing $H^2(\sigma)$ as a self-adjoint operator and project onto the positive part of the spectrum for every σ. The practical problem that arises here is that we do not know the spectrum of the physical Hamiltonian and hence we cannot follow this way. Therefore, we choose the same strategy as in [5] and consider an absolute value under the square root and quantize

$$\mathbf{H}_{\mathrm{phys}} = \int_{\mathcal{S}} d^3\sigma \sqrt{|-2\sqrt{Q}C^{\mathrm{geo}} + 2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C_j^{\mathrm{geo}}C_j^{\mathrm{geo}}}|(\sigma)}. \tag{405}$$

In the classical regime the expressions for $\mathbf{H}_{\mathrm{phys}}$ are identical, since we know that $|-2\sqrt{Q}C^{\mathrm{geo}} + 2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C_j^{\mathrm{geo}}C_j^{\mathrm{geo}}}| = -2\sqrt{Q}C^{\mathrm{geo}} + 2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C_j^{\mathrm{geo}}C_j^{\mathrm{geo}}} \geq 0$ and in the quantum theory we ensure a well defined expression under the square root by taking the absolute value. The general strategy for the quantization within LQG one follows is to introduce a regulator by means of which a regularization of $\mathbf{H}_{\mathrm{phys}}$ can be found. Afterwards one shows that in the limit where the regulator is removed one ends up with a well defined expression for the physical Hamiltonian operator $\hat{\mathbf{H}}_{\mathrm{phys}}$. As mentioned before in contrast to other physical Hamiltonians that have been quantized so far, in our case $\mathbf{H}_{\mathrm{phys}}$ is no longer covariant at the observable level because the summation is performed outside the square root in $\mathbf{H}_{\mathrm{phys}}$ and thus we need to introduce a different regularization procedure here. As far as the first term under the square root is considered, we can quantize it by applying a regularization that has already been discussed in the literature for the Hamiltonian constraint in [138] and for the volume operator in [114]. To quantize the second term under the square root as a first step we rewrite it in terms of densitized triads. This results in

$$\begin{aligned}\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C_j^{\mathrm{geo}}C_j^{\mathrm{geo}}} &= \sum_{j=1}^{3}\sqrt{QQ^{jj}C_j^{\mathrm{geo}}C_j^{\mathrm{geo}}} = \sum_{j=1}^{3}\sqrt{\frac{Q\delta^{JK}E_J^jE_K^jF_{jk}^LF_{j\ell}^ME_L^kE_M^\ell}{Q}} \\ &= \sum_{j=1}^{3}\sqrt{E_J^jE_K^jF_{jk}^LF_{j\ell}^ME_L^kE_M^\ell\delta^{JK}} = \sum_{j=1}^{3}\sqrt{F_{jk}^LE_J^jE_L^kF_{j\ell}^ME_K^jE_M^\ell\delta^{JK}} \\ &= \sum_{j=1}^{3}\sqrt{O_J^{(j)}O_K^{(j)}\delta^{JK}},\end{aligned} \tag{406}$$

where we introduced the quantities $O_J^{(j)} := F_{jk}^LE_J^jE_L^k$ (no summation over j) and we used that $Q^{ij} = \frac{\delta^{JK}E_J^iE_K^j}{Q}$, $Q(E) := \det(Q_{ij}(E))$, $C_j^{\mathrm{geo}} = F_{jk}^LE_L^k$ with scalar field manifold indices $i, j, \ldots$ and su(2) Lie algebra indices $I, J, \ldots$. At the classical level the order of the curvature F and the densitized triads E is irrelevant but at the quantum level it is important that F is ordered to the left in order to avoid the creation of infinitely many loops at the vertices of a given graph when the operator acts on the corresponding cylindrical function. In the next section we will discuss the regularization of the physical Hamiltonian in detail.

9.6.1 Regularization of $\mathbf{H}_{\mathrm{phys}}$

For the regularization of $\mathbf{H}_{\mathrm{phys}}$ we will introduce a point splitting regularization along the lines of [9] where it was applied to quantize the volume operator of LQG. For this purpose we need to introduce a characteristic function associated with some geometrical objects that we denote by $\bigstar$. In principal we can make an arbitrary choice for such geometrical objects, however usually in the existing literature cubes or tetrahedra have been chosen. The only difference between different choices for $\bigstar$ will be a constant global factor, called the regularization constant $c_\bigstar$. This constant is involved in the volume of the considered objects, i.e. $\mathrm{vol}(\bigstar) = c_\bigstar \epsilon^3$, where $\epsilon > 0$ is the basic length of the object under consideration. For example, for a cube denoted by $\square$ we have $c_\square = 1$ and for a tetrahedron denoted by $\triangle$ we get $c_\triangle = \frac{\sqrt{2}}{12}$. To keep our presentation simple and to be able to compare our results with already existing results we will use tetrahedra in the embedded LQG case and cubes for the AQG framework. The reason for these choices is that then we can carry over already existing quantization techniques for C^{geo} [5, 8] to the case of our physical Hamiltonian. Before we perform the point splitting, we write $\mathbf{H}_{\mathrm{phys}}$ as

$$\mathbf{H}_{\mathrm{phys}} = \int\limits_{\mathcal{S}} d^3p \sqrt{|-2\sqrt{Q}C^{\mathrm{geo}} + 2\sum_{j=1}^{3}\sqrt{O_J^{(j)}O_K^{(j)}\delta^{JK}}|(p)}, \tag{407}$$

where $p := \sigma$ denotes the points of the scalar manifold $\mathcal{S}$ from now on. For the regularization of $O_J^{(j)}$ we will consider a point splitting regularization for the two densitized triads and the curvature similar to the case of the volume operator where a product of three densitzed triads is involved. Later we will reexpress the curvature in terms of holonomies as usually done in LQG. Let us discuss the individual steps in detail. For simplicity we discuss the case for $j = 1$ first, the remaining three cases work similar. Applying the point splitting we regularize $O_J^{(1)}$ as follows

$$\begin{aligned} O_J^{(1)}(p) &= \lim_{\triangle'\triangle\to 0} \frac{1}{\mathrm{vol}(\triangle')\mathrm{vol}(\triangle)} \int\limits_{\mathcal{S}} d^3y\, \chi_{\triangle'}(p,y) F_{1k}^M(y) E_J^1(y) \int\limits_{\mathcal{S}} d^3x\, \chi_\triangle(p,x) E_M^k(x) \\ &=: \lim_{\triangle'\triangle\to 0} O_J^{(1)}(p,\triangle',\triangle). \end{aligned} \tag{408}$$

Here $\chi_\triangle(p,x)$ denotes the characteristic function of a tetrahedron $\triangle$ with the limit $\lim\limits_{\triangle\to 0}\frac{\chi_\triangle(p,x)}{\mathrm{vol}(\triangle)} = \delta^{(3)}(p,x)$. Due to the Poisson algebra of the Ashtekar connection and the densitized triad which has the form $\{A_i^I(x), E_J^j(y)\} = \frac{\kappa\beta}{2}\delta_i^j\delta_J^I\delta^{(3)}(x,y)$ the operator corresponding to $E_J^j(x)$ can be represented by

$$\hat{E}_J^j(x) = -i\frac{\ell_P^2}{2}\frac{\delta}{\delta A_j^J(x)} \tag{409}$$

with the Planck length $\ell_P = \sqrt{\hbar\kappa}$ and we set $\beta = 1$ for simplicity. Given this, we can define a regularized flux operator by

$$\begin{aligned} \hat{E}_J^j(p,\triangle) &:= \frac{1}{\mathrm{vol}(\triangle)} \int\limits_{\mathcal{S}} \mathrm{d}^3x\, \chi_\triangle(p,x) \hat{E}_J^j(x) \\ &= -i\frac{\ell_P^2}{2}\frac{1}{\mathrm{vol}(\triangle)} \int\limits_{\mathcal{S}} \mathrm{d}^3x\, \chi_\triangle(p,x) \frac{\delta}{\delta A_j^J(x)}. \end{aligned} \tag{410}$$

Then we reexpress the regularized operator $O_J^{(1)}(p,\triangle',\triangle)$ as

$$\hat{O}_J^{(1)}(p,\triangle',\triangle) = \frac{(-i)^2\ell_P^4}{4}\frac{1}{\mathrm{vol}(\triangle')\mathrm{vol}(\triangle)} \int\limits_{\mathcal{S}} d^3y\, \chi_{\triangle'}(p,y) F_{1k}^M(y) \frac{\delta}{\delta A_1^J(y)} \int\limits_{\mathcal{S}} d^3x\, \chi_\triangle(p,x) \frac{\delta}{\delta A_k^M(x)}. \tag{411}$$

What we still have to analyze is whether the limit in which the regulator is removed leads to a well defined expression for $\hat{\mathbf{H}}_{\rm phys}$. For this purpose we will discuss in detail the action of $\hat{O}^{(1)}_J(p,\triangle',\triangle)$ on cylindrical functions and how the limit can be performed.

9.6.2 Action of $\hat{O}^{(j)}_J(p,\triangle',\triangle)$ on Cylindrical Functions

For analyzing the action of the regularized operator $\hat{O}^{(j)}_J(p,\triangle',\triangle)$ on a generic cylindrical function f_γ, we first compute the action of the regularized flux operator on f_γ. Afterwards we will discuss how the curvature can be regularized and expressed in terms of holonomy operators. We obtain for the action of the regularized flux operator on a generic cylindrical function f_γ

$$
\begin{aligned}
\hat{E}^j_J(p,\triangle)f_\gamma(h_e[A]) &= -i\frac{\ell_P^2}{2}\frac{1}{\mathrm{vol}(\triangle)}\int\limits_{\mathcal{S}} \mathrm{d}^3x\,\chi_\triangle(p,x)\frac{\delta h_e}{\delta A^J_j(x)}\frac{\delta}{\delta h_e}f_\gamma \\
&= +i\frac{\ell_P^2}{2}\frac{1}{\mathrm{vol}(\triangle)}\sum_{e\in E(\gamma)}\int\limits_0^1 \mathrm{d}t\,\chi_\triangle(p,e(t))\dot{e}^j(t)\frac{1}{2}\mathrm{Tr}\Big([h_e(0,t)\tau_J h_e(t,1)]\,\frac{\delta}{\delta h^T_e(0,1)}\Big)f_\gamma,
\end{aligned}
\tag{412}
$$

where we parametrize an edge e by $e:[0,1]\to\mathcal{S},\ t\mapsto e(t)$ and $\tau_J=i\sigma_J$ with $\sigma_J,\ J=1,2,3,$ being the Pauli matrices. We used the notation $f_\gamma=f_\gamma(h_e[A])$ to emphasize the dependence of a cylindrical function on the holonomies and the dependence of the latter on the connections. Now we can also apply the second part of the regularized operator leading to an action of $\hat{O}^{(j)}_J(p,\triangle',\triangle)$ on f_γ given by

$$
\begin{aligned}
\hat{O}^{(1)}_J(p,\triangle',\triangle)f_\gamma =& \frac{(+i)^2\ell_P^4}{4}\frac{1}{\mathrm{vol}(\triangle')}\frac{1}{\mathrm{vol}(\triangle)} \\
&\Big\{\sum_{e,e'\in E(\gamma)}\int\limits_0^1\mathrm{d}t'\int\limits_0^1\mathrm{d}t\,F^M_{1m}(e'(t'))\,\chi_{\triangle'}(p,e'(t'))\chi_\triangle(p,e(t))\dot{e}'^1(t')\dot{e}^m(t) \\
&\frac{1}{4}\mathrm{Tr}\Big([h_{e'}(0,t')\tau_J h_{e'}(t',1)]\,\frac{\delta}{\delta h^T_{e'}(0,1)}\Big)\,\mathrm{Tr}\Big([h_e(0,t)\tau_M h_e(t,1)]\,\frac{\delta}{\delta h^T_e(0,1)}\Big) \\
&+\sum_{e\in E(\gamma)}\int\limits_0^1\mathrm{d}t\int\limits_0^1\mathrm{d}t'\,F^M_{1m}(e(t'))\,\chi_{\triangle'}(p,e(t'))\chi_\triangle(p,e(t))\dot{e}^1(t')\dot{e}^m(t) \\
&\Big[\frac{1}{4}\Theta(t',t)\mathrm{Tr}\Big([h_e(0,t')\tau_J h_e(t',t)\tau_M h_e(t,1)]\,\frac{\delta}{\delta h^T_e(0,1)}\Big) \\
&+\frac{1}{4}\Theta(t,t')\mathrm{Tr}\Big([h_e(0,t)\tau_M h_e(t,t')\tau_J h_e(t',1)]\,\frac{\delta}{\delta h^T_e(0,1)}\Big)\Big]\Big\}f_\gamma,
\end{aligned}
\tag{413}
$$

where we again stick to the case $j=1$ here and $E(\gamma)$ denotes the set of all edges of the graph γ. In the next step we will discuss how the curvature term can be regularized. For this purpose we write it in a more convenient way by introducing for an associated tangent vector of a given edge $e^1(t)$ the following notation:

$$
\dot{e}^a_{(1)} := \delta^a_1\dot{e}^1(t).
\tag{414}
$$

This has the advantage that we can express the curvature as

$$
F^M_{1m}(e'(t'))\dot{e}'^1(t')\dot{e}^m(t) = F^M_{nm}(e'(t'))\dot{e}'^n_{(1)}(t')\dot{e}^m(t)
\tag{415}
$$

and similarly for the remaining cases $j = 2, 3$. Considering this we can rewrite $\hat{O}^{(j)}_J(p, \triangle, \triangle')f_\gamma$ as

$$\begin{aligned}
\hat{O}^{(j)}_J(p, \triangle', \triangle)f_\gamma = & \frac{(+i)^2\ell_P^4}{4}\frac{1}{\mathrm{vol}(\triangle')}\frac{1}{\mathrm{vol}(\triangle)} \qquad (416) \\
& \Bigg\{ \sum_{e,e'\in E(\gamma)} \int_0^1 \mathrm{d}t' \int_0^1 \mathrm{d}t\, F^M_{am}(e'(t'))\, \chi_{\triangle'}(p, e'(t'))\chi_\triangle(p, e(t))\dot{e}'^a_{(j)}(t')\dot{e}^m(t) \\
& \frac{1}{4}\mathrm{Tr}\bigg([h_{e'}(0, t')\tau_J h_{e'}(t', 1)]\, \frac{\delta}{\delta h^T_{e'}(0, 1)}\bigg)\, \mathrm{Tr}\bigg([h_e(0, t)\tau_M h_e(t, 1)]\, \frac{\delta}{\delta h^T_e(0, 1)}\bigg) \\
& + \sum_{e\in E(\gamma)} \int_0^1 \mathrm{d}t \int_0^1 \mathrm{d}t'\, F^M_{am}(e(t'))\, \chi_{\triangle'}(p, e(t'))\chi_\triangle(p, e(t))\dot{e}^a_{(j)}(t')\dot{e}^m(t) \\
& \bigg[\frac{1}{4}\Theta(t', t)\mathrm{Tr}\bigg([h_e(0, t')\tau_J h_e(t', t)\tau_M h_e(t, 1)]\, \frac{\delta}{\delta h^T_e(0, 1)}\bigg) \\
& + \frac{1}{4}\Theta(t, t')\mathrm{Tr}\bigg([h_e(0, t)\tau_M h_e(t, t')\tau_J h_e(t', 1)]\, \frac{\delta}{\delta h^T_e(0, 1)}\bigg)\bigg] \Bigg\} f_\gamma,
\end{aligned}$$

where again no summation over j is taken into account.

9.6.3 Regularization of $\sqrt{Q}C^{\mathrm{geo}}$ and its Action on Cylindrical Functions

As discussed above for the first term under the outer square root that involves the volume $\sqrt{Q}$ as well as the geometric part of the Hamiltonian constraint C^{geo} we will carry over existing results from the literature where the quantization of both operators has already been presented. In order to be able to perform the limit for both parts of the regularized $\mathbf{H}_{\mathrm{phys}}$ we will use the same strategy that was for instance followed in [1]. We introduce the following regularized quantities $\sqrt{Q}(p, \triangle)$ and $C^{\mathrm{geo}}(p, \triangle')$ defined through

$$\begin{aligned}
\sqrt{Q}(p) &:= \lim_{\triangle\to 0} \sqrt{Q}(p, \triangle) = \lim_{\triangle\to 0} \frac{1}{\mathrm{vol}(\triangle)} \int d^3x\, \sqrt{Q}(x)\chi_\triangle(p, x) \qquad (417) \\
C^{\mathrm{geo}}(p) &:= \lim_{\triangle'\to 0} C^{\mathrm{geo}}(p, \triangle') = \lim_{\triangle'\to 0} \frac{1}{\mathrm{vol}(\triangle')} \int d^3y\, C^{\mathrm{geo}}(y)\chi_{\triangle'}(p, y)
\end{aligned}$$

The action of their corresponding regularized operator product on cylindrical functions yields

$$\widehat{\sqrt{Q}}(p, \triangle)\widehat{C}^{\mathrm{geo}}(p, \triangle'))f_\gamma = \frac{1}{\mathrm{vol}(\triangle')\mathrm{vol}(\triangle)} \int d^3x \int d^3y\, \chi_\triangle(p, x)\chi_{\triangle'}(p, y)\widehat{\sqrt{Q}}_x\widehat{C}^{\mathrm{geo}}_y f_\gamma, \quad (418)$$

where $\widehat{\sqrt{Q}}_x, \widehat{C}^{\mathrm{geo}}_y$ denote the usual regularizations of the volume and the geometric Hamiltonian constraint that can for instance be found in [138] and [114]. In the next section we will discuss in detail how the limit of this regularized operator can be performed and how this can be used to finally define an operator for the physical Hamiltonian $\mathbf{H}_{\mathrm{phys}}$.

9.6.4 Performing the Limit of the Regularized Physical Hamiltonian

Let us start with discussing the limit for the regularized operator $\hat{O}^{(j)}(p, \triangle', \triangle)$. Due to the characteristic functions that are involved in the regularized operator, we realize that the first part of the operator involving the sum $\sum_{e,e'}$ will only contribute if e, e' have a point of intersection that we denote by p. In case they do not intersect, we can shrink $\triangle', \triangle$ appropriately to some small but finite region and both characteristic functions have support only in a neighborhood of p. Hence, if the edges do not intersect the first part vanishes identically. Let us assume that p is the point of intersection of e, e' at parameter values t_0, t_0'. For the reason that by assumption the edges are not self-intersecting t_0, t_0' are unique. We parametrize the edges as

$$e(t) = p + c(t - t_0), \quad e'(t') = p + c'(t' - t_0'), \tag{419}$$

where c, c' are analytic functions which vanish at $t - t_0 = 0$, respectively $t' - t_0' = 0$. Since e, e' must intersect at p it follows that $p = v = e \cap e'$ must be a common vertex of the edges. By assumption edges can only intersect at their beginning or final points. Without loss of generality we are able to choose an adapted graph γ in such a way that it will be possible to classify each edge as an edge of either type up or type down, respectively either type in or type out. If this is not directly given we can subdivide edges appropriately such that we are in this situation. Further, we divide the edges in such a way that they all have outgoing orientation with respect to a vertex v, which is also equal to the intersection point, such that the flux operators can entirely be expressed in terms of right invariant vector fields. In this case the edges intersect in their beginning point and thus the unique value of t_0, t_0' is given by $t_0 = t_0' = 0$. The general structure of the individual terms in the action of $\hat{O}^{(j)}(p, \triangle', \triangle)$ is of the form $\int dt \int dt' g(t')h(t)f_\gamma$ for appropriately chosen functions g and h. Taking the discussion above into account in the limit where the tetrahedra $\triangle$ become smaller and smaller we can expand the individual terms in the action in powers of ϵ according to:

$$\int_0^1 dt \int_0^1 dt' g(t')h(t)f_\gamma = \left(g(0)h(0)\frac{\epsilon^2}{4} + o(\epsilon^2) \right) f_\gamma, \tag{420}$$

where the limit $\triangle \to 0$ corresponds to $\epsilon \to 0$ because $\mathrm{vol}(\triangle) = c_\triangle \epsilon^3$. Note that the factor of $\frac{1}{4}$ is due to the fact that $\int_{\mathbb{R}_+} dt\delta(0,t) \int_{\mathbb{R}_+} dt'\delta(0,t') = \frac{1}{4}$. Additionally, we assumed that the functions g, h have only support in an interval ϵ which is given due to the characteristic functions involved. If we apply this kind of expansion to the action of $\hat{O}^{(j)}(p, \triangle', \triangle)$, we will end up with

$$\begin{aligned}
\hat{O}_J^{(j)}(p, \triangle', \triangle) f_\gamma = {} & \frac{(+i)^2 \ell_P^4}{4} \frac{1}{c_{\triangle'} c_\triangle \epsilon^6} \\
& \Bigg\{ \sum_{e,e' \in E(\gamma)} \frac{\epsilon^2}{4} \Big(F^M_{am}(e'(0))\, \chi_{\triangle'}(p, e'(0)) \chi_\triangle(p, e(0)) \dot{e}'^a_{(j)}(0) \dot{e}^m(0) \\
& \frac{1}{4} \mathrm{Tr}\Big([\tau_J h_{e'}(0,1)] \frac{\delta}{\delta h^T_{e'}(0,1)} \Big) \mathrm{Tr}\Big([\tau_M h_e(0,1)] \frac{\delta}{\delta h^T_e(0,1)} \Big) \Big) \\
& + \sum_{e \in E(\gamma)} \frac{\epsilon^2}{4} \Big(F^M_{am}(e(0))\, \chi_{\triangle'}(p, e(0)) \chi_\triangle(p, e(0)) \dot{e}^a_{(j)}(0) \dot{e}^m(0) \\
& \Big[\frac{1}{4} \mathrm{Tr}\Big([\tau_J \tau_M h_e(0,1)] \frac{\delta}{\delta h^T_e(0,1)} \Big) \\
& + \frac{1}{4} \mathrm{Tr}\Big([\tau_M \tau_J h_e(0,1)] \frac{\delta}{\delta h^T_e(0,1)} \Big) \Big) \Big] + o(\epsilon^2) \Bigg\} f_\gamma,
\end{aligned} \tag{421}$$

where we used that $\Theta(0,0) = 1$ as well as $h_e(0,0) = \mathbb{1}_{\mathrm{SU}(2)}$. For the approximation of the integrals we did not compute the terms of order ϵ^3 or higher explicitly here because these terms will vanish anyway in the limit where the regulator is removed. We can rewrite the second sum over the edges in a more compact form, if we introduce the anti-commutator $\{\tau_J, \tau_M\}_+$ and obtain

$$\begin{aligned}\hat{O}_J^{(j)}(p,\triangle',\triangle)f_\gamma &= \frac{(+i)^2\ell_P^4}{4}\frac{1}{c_{\triangle'}c_\triangle\epsilon^6} \\ &\Bigg\{\sum_{e,e'\in E(\gamma)}\frac{\epsilon^2}{4}\Big(F_{am}^M(e'(0))\,\chi_{\triangle'}(p,e'(0))\chi_\triangle(p,e(0))\dot{e}'^a_{(j)}(0)\dot{e}^m(0) \\ &\frac{1}{4}\mathrm{Tr}\Big([\tau_J h_{e'}(0,1)]\,\frac{\delta}{\delta h_{e'}^T(0,1)}\Big)\,\mathrm{Tr}\Big([\tau_M h_e(0,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Big)\Big) \\ &+\sum_{e\in E(\gamma)}\frac{\epsilon^2}{4}\Big(F_{am}^M(e(0))\,\chi_{\triangle'}(p,e(0))\chi_\triangle(p,e(0))\dot{e}^a_{(j)}(0)\dot{e}^m(0) \\ &\Big[\frac{1}{4}\mathrm{Tr}\Big([\{\tau_J,\tau_M\}_+ h_e(0,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Big)\Big] + o(\epsilon^2)\Bigg\}f_\gamma.\end{aligned} \tag{422}$$

Our next steps involve to replace the curvature by appropriate holonomy operators and to use the properties of the Pauli matrices to rewrite the anti-commutator in a convenient way. From our discussion above we know that $e(0) = e'(0) = v$ thus the curvature is evaluated at the vertices v in all terms. Similarly, we can replace $e(0), e'(0)$ by v in all characteristic functions. Using the expansion of a loop $\alpha_{e'(j)e}$ in powers of ϵ we have

$$h_{\alpha_{e'_{(j)}e}} = \mathbb{1}_{\mathrm{SU}(2)} + \epsilon^2 F_{ab}^J(v)\dot{e}'^a_{(j)}(0)\dot{e}^b(0)\frac{\tau_J}{2} + o(\epsilon^2) \tag{423}$$

and it is simple to show that the following identity holds:

$$F_{ab}^M(v)\dot{e}'^a_{(j)}(0)\dot{e}^b(0) = -\frac{1}{\epsilon^2}\mathrm{Tr}\Big(h_{\alpha_{e'_{(j)}e}}\tau^M\Big). \tag{424}$$

The anti-commutator satisfies $\{\tau_J, \tau_M\}_+ = -2\delta_{JM}\mathbb{1}_{\mathrm{SU}(2)}$. Reinserting both into eq. (422) we end up with

$$\begin{aligned}\hat{O}_J^{(j)}(p,\triangle',\triangle)f_\gamma &= \frac{(+i)^2\ell_P^4}{4}\frac{1}{c_{\triangle'}c_\triangle\epsilon^6} \\ &\Bigg\{\sum_{e,e'\in E(\gamma)}(-1)\frac{1}{4}\Big(\mathrm{Tr}\Big(h_{\alpha_{e'_{(j)}e}}\tau^M\Big)\,\chi_{\triangle'}(p,v)\chi_\triangle(p,v) \\ &\frac{1}{4}\mathrm{Tr}\Big([\tau_J h_{e'}(0,1)]\,\frac{\delta}{\delta h_{e'}^T(0,1)}\Big)\,\mathrm{Tr}\Big([\tau_M h_e(0,1)]\,\frac{\delta}{\delta h_e^T(0,1)}\Big)\Big) \\ &+\sum_{e\in E(\gamma)}(-1)\frac{1}{4}\Big(\mathrm{Tr}\Big(h_{\alpha_{e_{(j)}e}}\tau^M\Big)\,\chi_{\triangle'}(p,v)\chi_\triangle(p,v) \\ &\Big[(-1)\frac{1}{2}\mathrm{Tr}\Big(\mathbb{1}_{\mathrm{SU}(2)}\delta_{JM}h_e(0,1)\frac{\delta}{\delta h_e^T(0,1)}\Big)\Big] + o(\epsilon^2)\Bigg\}f_\gamma.\end{aligned} \tag{425}$$

To further rewrite the action of the operator we introduce the right invariant vector fields X_0^e and X_L^e associated with an edge e by

$$\begin{aligned}X_0^e &:= \mathrm{T}r\Big(\tau_0 h_e(0,1)\frac{\delta}{\delta h_e^T(0,1)}\Big), \\ X_L^e &:= \mathrm{T}r\Big(\tau_L h_e(0,1)\frac{\delta}{\delta h_e^T(0,1)}\Big),\end{aligned} \tag{426}$$

where L runs from $1, \dots 3$, and we also include the 2×2 unity matrix $\sigma_0 = \mathbb{1}_{\mathrm{SU}(2)}$, that is $\tau_0 := i\sigma_0$. Then τ_0 and τ_J, $J = 1, 2, 3$, are the generators of the group U(2), since every element of U(2) can be written as the exponential of a Hermitian 2×2 matrix which is equal to $\exp\left(a\sigma_0 + b^J \sigma_J\right)$ with $a, b^J \in \mathbb{R}$. In this context we can understand X_0^e, X_L^e as right invariant vector fields associated with U(2).

For the reason that the edges have to intersect in a common vertex v, we can rewrite both sums over edges as a sum over all vertices and a sum over all edges meeting at these vertices. Hence, the action of $\hat{O}_J^{(j)}(p, \triangle', \triangle)$ on f_γ reads

$$\begin{aligned}\hat{O}_J^{(j)}(p, \triangle', \triangle) f_\gamma = -\frac{(+i)^2 \ell_P^4}{4} \frac{1}{c_{\triangle'} c_\triangle \epsilon^6} & \\ \Bigg\{ \frac{1}{16} \sum_{v \in V(\gamma)} \sum_{e \cap e' = v} \chi_{\triangle'}(p, v) \chi_\triangle(p, v) \operatorname{Tr}\Big(h_{\alpha_{e'_{(j)} e}} \tau^M\Big) X_J^{e'} X_M^e & \\ + \frac{i}{8} \delta_{JM} \sum_{v \in V(\gamma)} \sum_{b(e) = v} \chi_{\triangle'}(p, v) \chi_\triangle(p, v) \operatorname{Tr}\Big(h_{\alpha_{e_{(j)} e}} \tau^M\Big) X_0^e + o(\epsilon^2) \Bigg\} f_\gamma. &\end{aligned} \tag{427}$$

In order to obtain the final operator for $\hat{\mathbf{H}}_{\text{phys}}$ we need to consider the limit where the regulator is removed explicitly, that is the limit in which the volume of all tetrahedra shrinks to zero or equivalently ϵ tends to zero. Without loss of generality we can choose $\triangle = \triangle' = \triangle'' = \triangle''' =: \triangle$ where $\triangle, \triangle', \triangle'', \triangle'''$ denote the tetrahedra associated to the regularization of the individual operators involved in $\hat{\mathbf{H}}_{\text{phys}}$ and perform all limits simultaneously. Then we can just consider the limit $\epsilon \to 0$. Formally, we have

$$\hat{\mathbf{H}}_{\text{phys}} f_\gamma := \lim_{\epsilon \to 0} \hat{\mathbf{H}}^\epsilon_{\text{phys}} f_\gamma. \tag{428}$$

With our discussion above, the total regularized physical Hamiltonian is given by

$$\begin{aligned}\hat{\mathbf{H}}_{\text{phys}} f_\gamma := \lim_{\epsilon \to 0} \int d^3p \Big[2 \Big| - \frac{\chi_\triangle^2(p, v)}{c_\triangle c_\triangle \epsilon^6} \frac{1}{2} \widehat{\sqrt{Q}}_v \hat{C}_v^{\text{geo}} & \\ + \sum_{j=1}^{3} \Big[\sum_{v \in V(\gamma)} \left(\frac{(+i)^2 \ell_P^4}{4} \right)^2 \frac{\chi_\triangle^4(p, v)}{c_\triangle^4 \epsilon^{12}} & \\ \Big(\frac{1}{16} \sum_{e \cap e' = v} \operatorname{Tr}\Big(h_{\alpha_{e'_{(j)} e}} \tau^M\Big) X_J^{e'} X_M^e + \frac{i}{8} \delta_{JM} \sum_{b(e) = v} \operatorname{Tr}\Big(h_{\alpha_{e_{(j)} e}} \tau^M\Big) X_0^e + o(\epsilon^2) \Big)^\dagger & \\ \Big(\frac{1}{16} \sum_{e'' \cap e''' = v} \operatorname{Tr}\Big(h_{\alpha_{e'''_{(j)} e''}} \tau^M\Big) X_K^{e'''} X_N^{e''} + \frac{i}{8} \delta_{KN} \sum_{b(e'') = v} \operatorname{Tr}\Big(h_{\alpha_{e''_{(j)} e''}} \tau^N\Big) X_0^{e''} \Big) + o(\epsilon^2) \Big) & \\ \delta^{JK} \Big]^{\frac{1}{2}} \Big| \Big]^{\frac{1}{2}} f_\gamma, &\end{aligned} \tag{429}$$

where we chose the operator ordering of $\hat{O}_J^{(j)}(p, \triangle', \triangle)$ and its adjoint in such a way that the square of this operator does not create an infinite number of holonomy loops at the vertices.

Now in the limit $\epsilon \to 0$ only at most one vertex will contribute because in this limit at most one vertex is contained in the volume of $\triangle$ if these $\triangle$'s are sufficiently small or equivalently if ϵ is small enough. Given this, we can take the powers of the characteristic functions first out of the inner square root and afterwards out of the remaining square root. In case we further use that these characteristic functions become δ-functions in that limit and also that all $o(\epsilon^2)$-terms vanish we finally obtain

$$\hat{\mathbf{H}}_{\mathrm{phys},\gamma} f_\gamma = \int d^3p\, \hat{\mathbf{h}}_{\mathrm{phys},\gamma}(p) f_\gamma \tag{430}$$

with

$$\hat{\mathbf{h}}_{\mathrm{phys},\gamma}(p) := \sum_{v\in V(\gamma)} \delta^{(3)}(p,v)\hat{\mathbf{h}}_{\mathrm{phys},\gamma,\mathrm{v}}, \tag{431}$$

where we added an extra index γ as a reminder of the graph dependence and chose a symmetric ordering of the term involving $\hat{C}^{\mathrm{geo}}_{\gamma,v}$ after performing the limit $\epsilon \to 0$. So $\hat{\mathbf{h}}_{\mathrm{phys},\gamma,\mathrm{v}}$ reads

$$\begin{aligned}\hat{\mathbf{h}}_{\mathrm{phys},\gamma,\mathrm{v}} := \Big[2\Big| - \frac{1}{2}\left(\widehat{\sqrt{Q}}_{\gamma,v}\hat{C}^{\mathrm{geo}}_{\gamma,v} + (\hat{C}^{\mathrm{geo}}_{\gamma,v})^\dagger\widehat{\sqrt{Q}}_{\gamma,v}\right) + \sum_{j=1}^{3}\Big[\left(\frac{(+i)^2\ell_P^4}{4}\right)^2 \delta^{JK} \\ \Big(\frac{1}{16}\sum_{e\cap e'=v}\mathrm{Tr}\Big(h_{\alpha_{e'(j)e}}\tau^M\Big)X^{e'}_J X^e_M + \frac{i}{8}\delta_{JM}\sum_{b(e)=v}\mathrm{Tr}\big(h_{\alpha_{e(j)e}}\tau^M\big)X^e_0\Big)^\dagger \\ \Big(\frac{1}{16}\sum_{e''\cap e'''=v}\mathrm{Tr}\Big(h_{\alpha_{e'''(j)e''}}\tau^M\Big)X^{e'''}_K X^{e''}_N + \frac{i}{8}\delta_{KN}\sum_{b(e'')=v}\mathrm{Tr}\Big(h_{\alpha_{e''(j)e''}}\tau^N\Big)X^{e''}_0\Big)\Big]^{\frac{1}{2}}\Big|\Big]^{\frac{1}{2}}.\end{aligned} \tag{432}$$

We will postpone a discussion about the action of the individual parts of this physical Hamiltonian operator to section 9.7 where we combine this discussion with a comparison to the physical Hamiltonian operator of the one Klein–Gordon scalar field model in [1]. Before doing so we will discuss some aspects of graph-modifying versus graph-preserving quantizations and afterwards show how the operator can be quantized using the framework of Algebraic Quantum Gravity [5].

9.6.5 Remarks on the Application of the LQG Framework

There is a conceptual difference when we perform an unreduced or reduced quantization of LQG as far as the spatial diffeomorphism group is considered. In the case of the unreduced quantization spatial diffeomorphism are understood as gauge transformations and one eliminates them via a Dirac quantization procedure. Now in the case of the reduced quantization we look for representations of the observable algebra whose elements are Dirac observables carrying tensor indices of the scalar field manifold. As a consequence, in the reduced case the spatial diffeomorphism group is no longer a gauge group but should be understood as active diffeomorphisms and hence a symmetry group, for more details see the discussion in [5]. Now due to the fact that the observable algebra can also be represented by the standard Ashtekar-Lewandowski representation in the reduced quantization the representation of the physical Hilbert space is chosen to be the standard kinematical representation used in the Dirac quantization approach. As shown in [139] spatially diffeomorphism invariant operators can only be implemented in a graph-preserving way in this representation. In [5] the physical Hamiltonian is also on the dust manifold a spatially diffeomorphism invariant quantity and this led the authors of [5] to the conclusion that the resulting physical Hamiltonian in this model must be quantized in a graph-preserving way. However, this constraint is absent in our model because as far as the scalar field manifold is considered $\mathbf{H}_{\mathrm{phys}}$ is not spatially diffeomorphism invariant and therefore $\mathbf{H}_{\mathrm{phys}}$ needs not necessarily to be quantized graph non-changing. If we would additionally require the operator to be graph-preserving and implement this by introducing similar projectors as has be done in [5], then we are in a situation where all contributions of the unusual second term are trivial for the following reason: In cases where the edge e does not point into one of the j-directions the way the loop is attached will change the underlying graph γ and hence these contributions will be projected out. If e points in one of the j-directions, then as discussed below the loop operator $h_{\alpha_{e_{(j)}e}}$ will become the identity operator and thus the trace involving this loop operator will vanish. Therefore, for a graph-preserving quantization the unusual second term does not contribute to the final action. A similar property can be found for the quantization of $\mathbf{H}_{\text{phys}}$ in the context of Algebraic Quantum Gravity that will briefly discussed in the next section.

9.6.6 Quantization of the Physical Hamiltonian in the AQG Framework

The idea of the Algebraic Quantum Gravity (AQG) framework is to quantize the dynamical operators completely at the algebraic level where no information about the embeddings of the graphs into the spatial manifold is known. This information is encoded in semiclassical states that can only be defined for a given but arbitrary choice of an embedding. Given these semiclassical states the classical limit of the dynamical operators can be computed and their algebraic quantization has to be chosen in such a way that their semiclassical limit has in lowest order in $\hbar$ the correct classical limit of canonical general relatvity. Hence, here this will be the guiding principle for choosing an operator at the algebraic level and as far as the semiclassical limit is concerned we use the former results of [5] to define the corresponding AQG operator for the four scalar field model analyzed in our work here. As in [5] we consider an AQG model of cubic topology which consists of an infinite algebraic graph with six valent vertices. We choose the orientation of all edges in such a way that all edges have outgoing orientation with respect to a vertex v. Using a similar notation to the one that was introduced in [3] we label the six edges by $e_j^\sigma(v)$, here σ stands for the positive $\sigma = +$ or negative direction $\sigma = -$ and $j = \{1, 2, 3\}$ denotes the edge e whose tangent vector points into the j-th direction. Furthermore we choose $\{e_1, e_2, e_3\}$ to be right oriented with respect to the orientation of the field manifold $\mathcal{S}$. Note that although we use the same symbol the coordinates σ^j of the dust manifold and the σ here are completely unrelated. In order to implement a quantization of the loop operator at the algebraic level in a graph-preserving way we use the notion of a ***minimal loop*** introduced in [5]. For this purpose we further define $e_j^+ := e_j(v)$ and $e_j^- := e_j(v - \hat{j})$ where $v - \hat{j}$ is a translation of the point v along one unit of the $\hat{j}$-axis while the other two directions do not change. Here we will parametrize the minimal loop α by i, σ, j, σ' and v denotes the vertex the minimal loop is attached to. Having introduced the definition of the edges above, we can then obtain a minimal loop by the composition of the edges in the following way

$$\alpha_{\{(i,\sigma,j,\sigma'),v\}} = e_i^\sigma(v) \circ e_j^{\sigma'}(v + \sigma\hat{i}) \circ (e_i^\sigma)^{-1}(v + \sigma'\hat{j}) \circ (e_j^{\sigma'})^{-1}(v). \tag{433}$$

The holonomy along the minimal loop is then given by

$$h_{\alpha_{\{(i,\sigma,j,\sigma'),v\}}} = h_{(i,\sigma),v} \circ h_{(j,\sigma'),v+\sigma\hat{i}} \circ h^{-1}_{(i,\sigma),v+\sigma'\hat{j}} \circ h^{-1}_{(j,\sigma'),v} =: h_{\alpha_\square}. \tag{434}$$

For a visualization of the notions for an AQG graph, see figure 1.

Notice that here h still denotes a SU(2) holonomy. With this graph-preserving quantization we immediately realize that the contribution of the second unusual term in the embedded case has a trivial contribution in AQG and therefore does not need to be considered in the final form of $\hat{\mathbf{H}}_{\text{phys}}$. This also synchronizes well with the fact in the AQG framework the operators are supposed to be embedding independent. In order to illustrate this point more in detail we consider in figure 2b as an example the following minimal loop

$$\alpha_{\{(j,+,j,+),v\}} = e_j^+(v) \circ e_{(j)}^+(v + \hat{j}) \circ (e_j^+)^{-1}(v + \hat{j}) \circ (e_{(j)}^+)^{-1}(v) = \text{Id}, \tag{435}$$

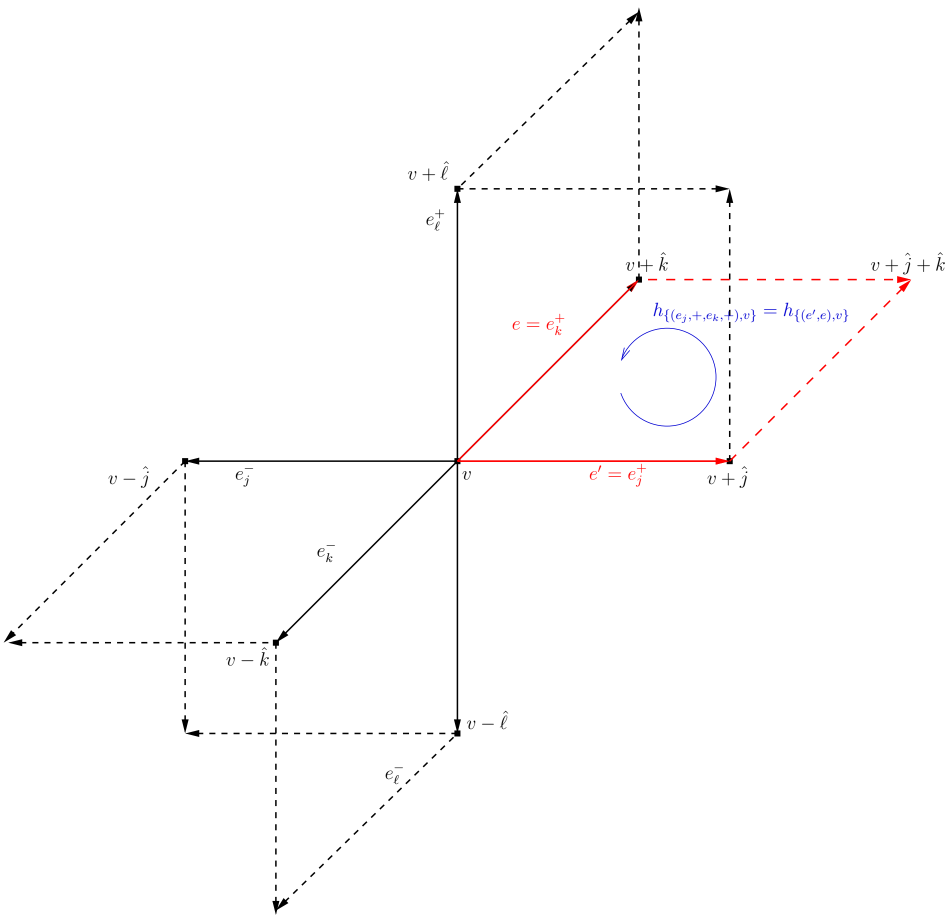


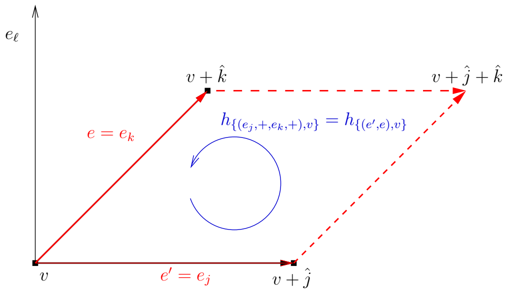
Figure 1: AQG cubic graph

where Id stands for the identity map, so that the holonomy along this loop becomes $h_{\alpha_{\{(j,+,(j),+),v\}}} = \mathbb{1}_{\mathrm{SU}(2)}$. Thus, we realize that in case of a cubic algebraic graph and a graph-preserving quantization the edges $e^\sigma_{(j)}$ and e^σ_j can always be identified. Hence, the operator in the AQG framework at each vertex takes the following form:

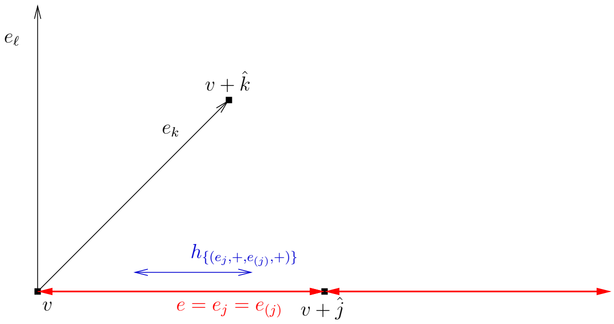
$$\hat{\mathbf{h}}_{\mathrm{phys},\gamma,\mathrm{v}} := \Big[2\Big| - \frac{1}{2}\left(\widehat{\sqrt{Q}}_{\gamma,v}\hat{C}^{\mathrm{geo}}_{\gamma,v} + \left(\hat{C}^{\mathrm{geo}}_{\gamma,v}\right)^\dagger \widehat{\sqrt{Q}}_{\gamma,v}\right) + \sum_{j=1}^{3}\Big[\left(\frac{(+i)^2\ell_P^4}{4}\right)^2 \delta^{JK}\left(\frac{1}{16}\right)^2 \tag{436}$$
$$\Big(\sum_{e\cap e'=v}\Big(\mathrm{Tr}\Big(h_{\alpha_{\{(j,\sigma',i,\sigma),v\}}}\tau^M\Big)X_{J,\{(j,\sigma'),v\}}X_{M,\{(i,\sigma),v\}}\Big)^\dagger$$
$$\Big(\mathrm{Tr}\Big(h_{\alpha_{\{(j,\sigma''',k,\sigma''),v\}}}\tau^N\Big)X_{K,\{(k,\sigma'''),v\}}X_{N,\{(\ell,\sigma''),v\}}\Big)\Big]^{\frac{1}{2}}\Big|\Big]^{\frac{1}{2}}$$

where the right invariant vector fields are given by $X^e_K = X^{e^\sigma_i}_K = X_{K,\{(i,\sigma),v\}}$ and we have

$$\hat{C}^{\mathrm{geo}}_{\gamma,v} = \frac{1}{24\ell_P^2}\sum_{i,j,k}\sum_{\sigma,\sigma',\sigma''=\pm}\sigma\sigma'\sigma''\epsilon^{ijk}\,\mathrm{Tr}\Big(h_{\alpha_{\{(i,\sigma,j,\sigma'),v\}}}h_{e_{\{(k,\sigma''),v\}}}\Big[h^{-1}_{e_{\{(k,\sigma''),v\}}},\hat{V}_{\gamma,v}\Big]\Big) \tag{437}$$



(a) First term



(b) Second term

Figure 2: Action of the first and the second term in $\hat{O}_J^{(j)}$ on a cubic AQG graph

with $\hat{V}_{\gamma,v}$ the volume operator for a graph γ , see also [5], given by

$$\hat{V}_{\gamma,v} = \sqrt{\hat{Q}}_{\gamma,v} = \ell_P^3 \sqrt{\left| \frac{1}{48} \sum_{i,j,k} \sum_{I,J,K} \sum_{\sigma,\sigma',\sigma''=\pm} \sigma\sigma'\sigma''\epsilon^{ijk}\epsilon^{IJK}\, X_{I,\{(i,\sigma),v\}} X_{J,\{(j,\sigma'),v\}} X_{K,\{(k,\sigma''),v\}} \right|}. \tag{438}$$

Then the physical Hamiltonian operator becomes

$$\hat{\mathbf{H}}_{\mathrm{phys},\gamma} f_\gamma = \sum_{v\in V(\gamma)} \hat{\mathbf{h}}_{\mathrm{phys},\gamma,\mathrm{v}} f_\gamma. \tag{439}$$

This finishes our discussion on the quantization of the physical Hamiltonian in the AQG framework.

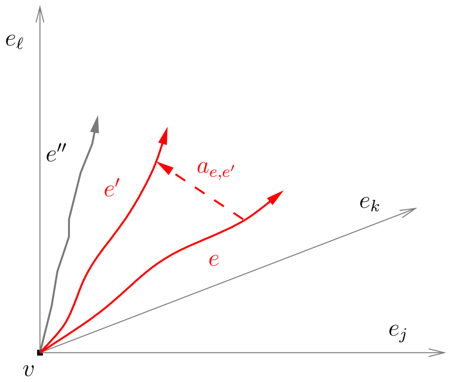
9.7 Comparison with the Model from [1]

Let us briefly discuss to what kind of contributions the operator in the LQG framework will lead if it acts on a generic spin network function. This also allows us to compare it to the physical Hamiltonian in [1] and analyze their differences in detail.

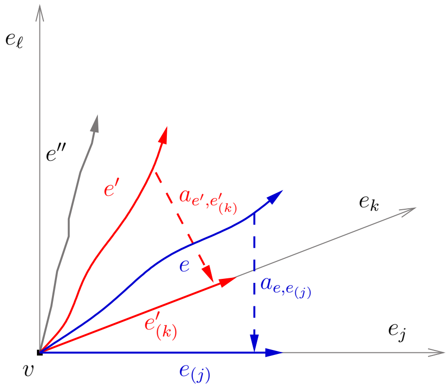
The first term under the square root in eq. (432) involving the volume operator as well as the geometric part of the Hamiltonian constraint operator is similar to the contributions that occur in the one Klein-Gordon scalar field model introduced in [1]. For that model an additional term that involves $Q^{jk}C_j^{\mathrm{geo}}C_k^{\mathrm{geo}}$ at the classical level is neglected because in that model the spatial diffeomorphism constraint is solved via Dirac quantization and thus the physical Hamiltonian needs to be implemented on the spatial diffeomorphism invariant Hilbert space $\mathcal{H}_{\mathrm{diff}}$. The operator version of the neglected term is expected to vanish on spatially diffeomorphism invariant states. The final physical Hamiltonian that one works with in [1] is of the form:

$$\widehat{\mathbf{H}}_{\mathrm{phys}} = \int d^3x \sqrt{-2\sqrt{\widehat{Q}}\widehat{C}^{\mathrm{geo}}}(x). \tag{440}$$

Let us now compare our physical Hamiltonian operator shown in eq. (432) to the one in [1] displayed above in eq. (440). A comparison of both models is possible according to the similarity of the first term under the square root in both models, despite that in our model the situation is different, since after the reduction with respect to the second class constraints we are left with



(a) Action of the first term in $\hat{O}_J^{(j)}$.



(b) Action of the second term in $\hat{O}_J^{(j)}$.

Figure 3: Action of $\hat{O}_J^{(j)}$ on LQG spin network functions

four reference fields for all constraints instead of one Klein–Gordon scalar field as a reference field for the Hamiltonian constraint. At the classical level the term $2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C_j^{\mathrm{geo}}C_j^{\mathrm{geo}}}$ can be understood as a contribution to the physical Hamiltonian density associated with the momentum density of the reference fields φ^j that would be absent in case where we consider only one instead of four reference fields. Thus, the fingerprint of the spatial reference fields encoded in $2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C_j^{\mathrm{geo}}C_j^{\mathrm{geo}}}$ at the classical level, caused by the dynamical coupling of this reference fields, also carries over to the quantum theory and yields to the remaining terms under the square root in eq. (432) corresponding the the quantization of the classical term $2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C_j^{\mathrm{geo}}C_j^{\mathrm{geo}}}$. Now the operator $\hat{O}_J^{(j)}$ whose square occurs under the second square root consists of a combination of right invariant vector fields and a loop holonomy operator. For a given vertex v of a graph γ associated to a given spin network function, there are two different contributions. The first one considers every pair of edges e, e' at v and acts with two right invariant vector fields $X_J^{e'}X_M^e$ onto them and afterwards attaches a loop along the edges e and e' to the graph γ, see figure 3a. The second contribution involves for each vertex v and every edge e attached to it an action of one right invariant vector field X_0^e . In this case the loop that acts afterwards goes along the edges e and the edge that one obtains by projecting the edge e onto the jth tangential direction, as can be seen in figure 3b. Note that this second contribution depends crucially on the embedding of the individual edges and is a contribution to the operator that is rather unusual. This can for instance be seen in the specific case where the tangent vector to e has a non-vanishing contribution only in one fixed j-direction. In this case the loop $h_{\alpha_{e(j)e}}$ is just the identity and since $\mathrm{Tr}(\tau^M) = 0$ the contribution of the second sum just vanishes identically. However, for a generic embedding of the edges with a tangent vector that has non-zero components in all j-directions the contribution from the second sum will in general be non-zero. Similar expressions occur in the regularization of the volume operator in [8, 9] and would also be involved in a point splitting regularization of the area operator. However, in these cases due to the specific structure of the volume and area operator, in particular both involve only covariant contractions, all terms of these kind vanish in the limit when the regulator is removed. For our physical Hamiltonian this is no longer true and the reason for this seems to be its non-covariant form at the level of observables, that is with respect to the scalar field manifold indices.

At first glance this seems unusual but as we show in appendix C, this is caused by the particular choice of gauge fixing associated with this model. As can be seen in the presentation in appendix C the induced shift vector associated with the choice of clocks in this model has at the observable level the form $N^k = \frac{1}{h(Q,P)} \sum_{j=1}^{3} \sqrt{Q}\sqrt{Q^{jj}}\delta_j^k$ which naturally explains the second embedding dependent term in the physical Hamiltonian.

Finally, let us mention that as in the models in [5, 12] the observable $C_j^{\rm geo}$ is a constant of motion with respect to the reference time τ, as can be seen by using the properties of the observable map. We have:

$$\frac{dC_j^{\rm geo}}{d\tau} = \{C_j^{\rm geo}(\sigma,\tau), \mathbf{H}_{\rm phys}\} = \{O^{(2)}_{\widetilde{c}_j,\widetilde{\varphi}^0}, O^{(2)}_{\widetilde{h},\widetilde{\varphi}^0}\} = O^{(2)}_{\{\widetilde{c}_j,\widetilde{h}\}^*} = O^{(2)}_{\{\widetilde{c}_j,\widetilde{h}\}} = 0. \tag{441}$$

Furthermore in the limit of vanishing momentum density of the reference fields φ^j as expected the model in [1] and our model here posses the same physical Hamiltonian and in this sense the generalized model introduced in this section can be understood as the corresponding four scalar field model associated with the model introduced in [1]. In the context of cosmology it can also be understood as the natural full Loop Quantum Gravity generalization of the APS-model in [24].

10 Conclusions

Large parts of this section have been published in [130]. We discussed the reduced phase space quantization in the context of Klein-Gordon scalar fields as reference matter. Such models can be understood as a natural generalization of the APS-model [24] in the framework of loop quantum cosmology to full Loop Quantum Gravity (LQG). The first model that was derived as a generalization along these lines is the model in [1], for which only one Klein-Gordon scalar field was considered. This allows to deparametrize the Hamiltonian constraint and use this Klein-Gordon scalar field as reference matter for the Hamiltonian constraint, whereas the three spatial diffeomorphism constraints are dealt with using Dirac quantization. If we instead choose to consider the spatial diffeomorphism constraints also in the context of a reduced phase space quantization, we will need three more additional reference fields. For this reason we presented in section 7 a model where we couple gravity to four Klein-Gordon scalar fields. We derived the reduced phase space of this model in terms of the corresponding Dirac observables and also computed the associated physical Hamiltonian which generates their dynamics. We have shown in section 7 that for such a model the reduced quantization program cannot be completed because we obtain a physical Hamiltonian which cannot be quantized in the context of LQG. The main reason for this is that infinitesimal spatial diffeomorphisms $C_j^{\rm geo}$ cannot be implemented as well defined operators in the standard LQG representation as explained in section 2.4. They occur in the combination $\delta^{jk}C_j^{\rm geo}C_k^{\rm geo}$ in the physical Hamiltonian that cannot be promoted to a well defined operator. We have discussed the technical details of this aspect at the end of section 7.5.

If we compare the model in section 7 to the one in [1], we will realize that this is an example for a case where Dirac quantization and reduced quantization lead to very different results. If we choose to quantize the spatial diffeomorphisms via Dirac quantization following [1], the quantization can be completed. In contrast if we just add three more Klein-Gordon scalar fields to the model and aim at performing a reduced phase space quantization, this quantization program cannot be completed because we cannot quantize the dynamics on the physical Hilbert space using the usual LQG representation. Hence, the Quantum Einstein Equations of such a model cannot be formulated.

Given this negative result for the four Klein-Gordon scalar fields model, we generalized this model in section 8. Likewise to the seminal dust model introduced in [25, 27] we considered a model that contains next to the four scalar fields that we want to use as reference fields for the spatial diffeomorphism and the Hamiltonian constraint additional scalar fields, where first six additional scalar fields were considered. The constraint stability analysis of this model showed that there exist second class constraints. Unfortunately, if we try to reduce the phase space with respect to these second class constraints, we will see that the model is not consistent. In order to make the secondary constraints vanish we either have to make a choice where several of the additional scalar fields have to vanish and there are not enough left to obtain a quantizable model or we have to choose $\varphi^i_n = 0$ which is not compatible with our gauge fixing we used in section 7 and section 9.

We go one step further and simplify this model in section 9 with the purpose to obtain a quantizable model where the spatial diffeomorphism constraints can then be treated via reduced phase space quantization. The number of additional scalar fields next to the four Klein-Gordon scalar fields reduces from six to three further scalar fields. As discussed in detail in section 9.3 this model possesses second class constraints. When we reduce with respect to the second class constraints, we obtain a model with only first class constraints that involves gravity and four additional scalar fields. The reference field for the Hamiltonian constraint φ^0 is a standard Klein-Gordon scalar field likewise to the model in [1]. However, the dynamics of the spatial reference field φ^j describe a generalized dynamics, since they are coupled to three additional scalar fields, whose degrees of freedom are reduced when performing the reduction with respect to the second class constraints. In sections 9.4 and 9.5 we derive the corresponding reduced phase space and present the explicit construction of Dirac observables as it was also done in sections 7.3 and 7.3. It turns out that this generalized model has a physical Hamiltonian that can be quantized using techniques of LQG, which is discussed in more detail at the end of section 9.5. For the reason that the resulting physical Hamiltonian has a form which slightly differs from the one in [1] and the one in the Brown-Kuchař dust models from [5], we present in section 9.6 in detail the regularization and quantization of the physical Hamiltonian operator. As can be seen from equation (402) at the end of section 9.5 the physical Hamiltonian density consists of two main contributions. One involves the gravitational part of the Hamiltonian constraint $C^{\rm geo}$ and for this term we used the already existing quantization in the literature. In the context of a usual LQG quantization we used the results in [138] and for the Algebraic Quantum Gravity (AQG) framework we considered the results from [5]. For the second contribution, whose form is determined by the choice of one conventional and three generalized Klein-Gordon scalar fields as reference matter and that involves the geometrical part of the spatial diffeomorphisms $C^{\rm geo}_j$, no quantization was available before. In section 9.6 we present a regularization for this second contribution, discuss how the regularized operator acts on spin network function and show that we obtain a well defined operator on the physical Hilbert space when the regulator is removed. It turns out that the final operator depends on the particular embedding of the graph. Furthermore we also illustrate how this second contribution can be quantized in the framework of AQG [5] as a corresponding algebraic graph-preserving operator. Interestingly, the possible problematic unusual term which explicitly depends on the embedding naturally becomes the identity operator in a graph-preserving quantization and therefore the quantization within an AQG model is straightforward.

As a consequence, including the generalized model, we have two models available that can be understood as equally justified generalizations of the APS-model to full LQG. Their main difference lies in the fact how the spatial diffeomorphism constraints are handled. The first one from

[1] is obtained in the Dirac quantization program as far as the spatial diffeomorphism constraints are concerned. The model presented in section 9 on the other hand uses a reduced phase space quantization either in usual LQG or in the AQG framework. By comparison of their physical Hamiltonians, as done in section 9.7, we get a first hint towards the question in which sense the final models will differ, if we either use Dirac or reduced phase space quantization to handle the diffeomorphism constraints. A next step is to work with these models and analyze how the different quantization procedure might influence physical properties of the dynamical models. Due to the technical complexity in the full theory, such an analysis is planned at the level of symmetry reduced models beyond the level of homogeneous and isotropic models for which the second contribution in the physical Hamiltonian, involving the spatial diffeomorphism constraints, just vanishes. This will be a topic for future research and might also give new insights on the role of chosen reference matter (clocks) in the context of a reduced phase space quantization of quantum gravity. As far as the discussion in [23] is concerned the new model introduced in this work extends the possible models of type I and can be used to formulate another dynamical model of the Quantum Einstein Equation in the context of LQG.

Part IV
Semiclassical Perturbation Theory

In this part we want to review and enlarge an approach to calculate expectation values in the complexifier coherent states introduced in [43, 44, 45], also described in section 18. The approach is denoted as ***semiclassical perturbation theory*** and was introduced in [4]. The gist is that in semiclassical perturbation theory we do not modify the semiclassical states to calculate the expectation values, instead we try to cast the operator into a form which allows us to calculate its expectation value approximately with predictable deviations from the exact value of its expectation value.

11 Short Review on Semiclassical Perturbation Theory

We review the fundamental ideas and basic tools of semiclassical perturbation theory based on the work presented in [4]. A motivation for the development of semiclassical perturbation theory was the question how to calculate expectation values of in general non-integer powers of the volume operator $\hat{V}_v^{4q}$, see section 2.3, at each vertex of a given graph in the complexifier coherent states $\psi := \psi_g^t$, see section 18, i.e. expressions of the form $\langle\psi, \hat{V}_v^{4q}, \psi\rangle$, where q is a fractional number whose range is usually determined by the operator under consideration. The expectation value $\langle\psi, \hat{V}_v^{4q}, \psi\rangle$ is not computable analytically, but the most important outcome of the development of semiclassical perturbation theory in [4] is that it can be replaced up to $\hbar^{k+1}$ corrections by

$$|\langle\psi, \hat{Q}_v, \psi\rangle|^{2q} \left[1 + \sum_{n=1}^{2k+1} (-1)^{n+1} \frac{q(1-q)\ldots(2k-q)}{n!} \left(\frac{\hat{Q}_v^2}{\langle\psi, \hat{Q}_v, \psi\rangle^2} - 1\right)^n\right]. \tag{442}$$

Here the operator $\hat{Q}_v$ is a polynomial in the flux operators which is related to $\hat{V}_v$ by $\hat{V}_v =^4 \sqrt{\hat{Q}_v^2}$. Its expectation value $\langle\psi, \hat{Q}_v, \psi\rangle$ is known in closed form, see [43, 44, 45, 46, 115, 118]. Moreover, semiclassical perturbation theory provides a technique to calculate much more general expectation values of polynomials in holonomy operators and functions of volume operators in the complexifier coherent states ψ, namely

$$\langle\psi|p_1(\hat{h})F_1(\hat{V}_{v_1})\ldots p_N(\hat{h})F_N(\hat{V}_{v_2})p_{N+1}(\hat{h})|\psi\rangle, \tag{443}$$

where the p_j, $j = 1, \ldots, N+1$, are polynomials in the holonomy operators along edges or loops connected to the vertices $v_1, \ldots, v_N$ of a given graph γ and the F_I, $I = 1, \ldots, N$, are operator valued functions of the volume operator $\hat{V}_{v_I}$ of the form $F_I(\hat{V}_{v_I}) = \left(\hat{Q}_v^2\right)^{q_I}$. The exponent q_I is equal to $q_I = \frac{m_I}{n_I}$ with m_I, n_I relatively prime and has the range $0 < q_I \leq \frac{1}{4}$. The restriction of the range of q_I comes in during the proof of the validity of the approximation. One's interest in this kind of more general expectation values is based on the fact that they are basic building blocks in the calculation of the expectation value of the Master constraint [5, 29, 30] or physical Hamiltonian constraint operator as discussed in part III. The idea to calculate the expectation values in eq. (443) goes as follows: First we define the bounded operator

$$\hat{x}_I := \frac{\hat{Q}_{v_I}^2}{\langle\psi, \hat{Q}_v\psi\rangle^2} - \hat{\mathbb{1}} \tag{444}$$

with $||\hat{x}_I|| \geq 1$ and re-express the operator valued functions $F_I(\hat{V}_{v_I})$ by

$$\begin{aligned} F_I(\hat{V}_{v_I}) &= |\langle\psi, \hat{Q}_v\psi\rangle|^{2q_I} \left(\hat{\mathbb{1}} + \hat{x}_I\right)^{q_I} \\ &=: |\langle\psi, \hat{Q}_v\psi\rangle|^{2q_I} f_I(\hat{x}_I). \end{aligned} \tag{445}$$

Naively, we can try to use the power series expansion of the function $f : [-1, \infty) \to \mathbb{R}$, $t \mapsto f(t)$ given by

$$f(t) = 1 + \sum_{n=1}^{\infty} \binom{q}{n} t^n \tag{446}$$

to obtain an approximation for eq. (445) and we actually will use this in the following. However, it is not obvious that we are allowed to use the power series expansion, since we are dealing here with operators and indeed, if we assume that we have a projection-valued measure $\hat{E}_I(t)$ associated with $\hat{x}_I$ and apply the spectral theorem, we can see that

$$f_I(\hat{x}_I) = \int_{-1}^{\infty} f_I(t) \mathrm{d}\hat{E}_I(t) = \int_{-1}^{\infty} \left[1 + \sum_{n=1}^{\infty} \binom{q}{n} t^n\right] \mathrm{d}\hat{E}_I(t) \neq \left[\hat{\mathbb{1}} + \sum_{n=1}^{\infty} \binom{q}{n} \hat{x}_I^n\right]. \tag{447}$$

The last equality does not hold, since the power series does not converge outside the open interval $t \in (-1, 1)$. Nevertheless, we will see in the end that the naive ansatz works in case that we calculate expectation values of the power series expansion with respect to complexifier coherent states in which the properties of the complexifier coherent states play a crucial role here. To see how this works, we insert the expansion for $F_I(\hat{V}_{v_I})$ in eq. (445) into the expectation value of products of p_j's and F_I's in eq. (443) which results in

$$\begin{aligned} &\langle\psi|p_1(\hat{h})F_1(\hat{V}_{v_1}) \ldots p_N(\hat{h})F_N(\hat{V}_{v_2})p_{N+1}(\hat{h})|\psi\rangle \\ &= \prod_{j=1}^{N} |\langle\psi, \hat{Q}_{v_j}\psi\rangle|^{2q_j} \langle\psi, p_1 [1 + f_1] p_2 [1 + f_2] \ldots [1 + f_N] p_{N+1}\psi\rangle \\ &=: \prod_{j=1}^{N} F_j^0 \left[\langle\psi, p_1 p_2 \ldots p_{N+1}\psi\rangle + R\right] \end{aligned} \tag{448}$$

with $f_i = \sum_{n=1}^{\infty} \binom{q}{n} \hat{x}_i^n$, $i = 1, \ldots, N$. Here $F_j^0 := \prod\limits_{j=1}^{N} |\langle\psi, \hat{Q}_{v_j}\psi\rangle|^{2q_j}$ and the remainder R is a linear combination of terms of the form

$$\langle\psi, p'_1 f_1 \ldots f_l p'_{l+1}\psi\rangle \tag{449}$$

with $l = 1, \ldots, N$ and the p'_j's are polynomials in the p_j's. The remaining task is now to find an approximation for the terms in eq. (449) as shown in [4].

For this purpose we use an estimate which is stated in Lemma 2.1 in [4], see appendix G, which says that for each $k \geq 0$ exists a $0 < \beta_k < \infty$ such that

$$f_{2k+1}(t) - \beta_k t^{2k+2} \leq f(t) \leq f_{2k+1}(t), \tag{450}$$

and we define

$$f_-(t) := f_{2k+1}(t) - \beta_k t^{2k+2} \quad \text{and} \quad f_+(t) := f_{2k+1}(t), \tag{451}$$

where $f_{2k+1}(t) = \sum_{n=0}^{2k+1} \binom{q}{n} t^n$ is the partial Taylor series of $f(t)$ in eq. (446) and the inequality is valid for all $t \geq -1$. Next we define

$$\bar{f} := \frac{(f_+(t) + f_-(t))}{2} = f_{2k+1}(t) - \frac{\beta_k}{2} t^{2k+2}, \qquad (452)$$
$$\triangle f := \frac{(f_+(t) - f_-(t))}{4} = \frac{\beta_k}{4} t^{2k+2}$$

in order to be able to apply Lemma 2.3 from [4], see appendix G, which states that we can estimate

$$|\Re(\langle\psi_1, f(\hat{x})\psi_2\rangle) - \Re(\langle\psi_1, \bar{f}(\hat{x})\psi_2\rangle)| \leq \langle\psi_1, \triangle f(\hat{x})\psi_1\rangle + \langle\psi_2, \triangle f(\hat{x})\psi_2\rangle, \qquad (453)$$

where $\Re(\langle\psi., .\psi\rangle)$ denotes the real part of the expectation value in consideration and an analogous estimate holds for the imaginary part $\Im(\langle\psi., .\psi\rangle)$. Notice that the expectation values of $\bar{f}$ and $\triangle f$ can be calculated by the methods of [43, 44, 45, 46, 115, 118]. The estimate in Lemma 2.3 will be applied to all of the f_j's.

To decrease the number of N non-computable expectation values to $N-1$ non-computable expectation values with the help of the inequality in eq. (453), one has to start with the f_i operator in the "middle" which is given by $f_{\lfloor (N+1)/2 \rfloor}$, where $\lfloor\rfloor$ denote the Gauss brackets. However, it can never be achieved that all resulting expectation values are computable, but the non-computable expectation values can be estimated by computable ones of higher order in $\hbar$ than the order in $\hbar$ one considers in the perturbation theory. After finitely many steps we receive a computable expression which contains only the $\bar{f}_i$'s and is an estimate for our expectation value in eq. (449) up to order $\hbar^k$. Additionally, there are a finite number of expectation values which still contain at most N of the f_i's plus at least $2l+1$ insertion of the operators $\triangle f_i$ and can due to the existence of the f_i's not be computed, at least analytically. For N even this looks like

$$\langle P'_1[\triangle F'_1]P'_2 \ldots P'_l[\triangle F'_l]P_1 F_1 P_2 \ldots F_{N/2} P_{N/2+1}\psi| \qquad (454)$$
$$[\triangle F'_{l+1}] \quad |P'_1[\triangle F'_1]P'_2 \ldots P'_l[\triangle F'_l]P_1 F_1 P_2 \ldots F_{N/2} P_{N/2+1}\rangle$$

with $P'_j,\ P_k \in \{p_i\}_{i=1,\ldots,N+1},\ F_k \in \{f_i\}_{i=1,\ldots,N}$ and $\Delta F'_j$ for $F'_j \in \{f_i\}_{i=1,\ldots,N}$. We display how for l sufficiently large eq. (454) can be estimated by a computable expression at least of order $\hbar^{k+1}$. First we use the overcompleteness of the coherent states and insert the resolution of identity, for details see eq. (3.16) in [45] or section 18, given by

$$\int_{G^{\mathbb{C}}} d\nu_t(g) |\psi^t_g\rangle\langle\psi^t_g| = \hat{\mathbb{1}} \qquad (455)$$

in between the P'_j's, respectively P_k's, F_k's and $\Delta F'_j$'s.

Then, one has a product of integrals $\int_{G^{\mathbb{C}}} d\nu_t(g)$ over expectation values of the form

$$\langle\psi_1, P\psi_2\rangle, \quad \langle\psi_1, \triangle F'\psi_2\rangle, \quad \langle\psi_1, F\psi_2\rangle, \qquad (456)$$

where $\psi_1 := \psi^t_{g_1}$ and $\psi_2 := \psi^t_{g_2}$ denote two different complexifier coherent states and we leave out the details, displayed in section 18, in the indices here, since we just want to roughly explain how the estimate works. As explicitly calculated in [44, 45] and [4] we have

$$\langle\psi_1, P\psi_2\rangle = \langle\psi_1, \psi_2\rangle \left[E_0(\psi_1, \psi_2) + \hbar E_1(\psi_1, \psi_2)\right], \qquad (457)$$
$$\langle\psi_1, \triangle F'\psi_2\rangle = \hbar^{k+1}\langle\psi_1, \psi_2\rangle \left[G'_0(\psi_1, \psi_2) + \hbar G'_1(\psi_1, \psi_2)\right],$$
$$|\langle\psi_1, F\psi_2\rangle| \leq \hbar^{-3}\widetilde{\langle\psi_1, \psi_2\rangle} \left[G_0(\psi_1, \psi_2) + \hbar G_1(\psi_1, \psi_2)\right],$$

where $E_0, E_1, G_0', G_1', G_0, G_1$ are of zeroth order in $\hbar$ and absolutely integrable against the measures ν_1, ν_2. The overlap function $\langle\psi_1, \psi_2\rangle$ is sharply peaked at $\psi_1 = \psi_2$ and so are the functions $E_0, E_1, G_0', G_1', G_0, G_1$. A tilde over an overlap function indicates that $\widetilde{\langle\psi_1, \psi_2\rangle}$ is a Gaussian with respect to the momentum, but not with respect to the position variables of the phase space. After performing the integration over ψ_2, which we merely symbolize here by writing $\int \ldots \mathrm{d}\psi_2$, there are only integrals of states of type ψ_1 left. Therefore, we set, up to at least first order corrections in $\hbar$,

$$\int \langle\psi_1, P\psi_2\rangle \, \mathrm{d}\psi_2 = \langle\psi_1, \psi_1\rangle \left[E_0(\psi_1, \psi_1) + \mathcal{O}(\hbar)\right], \tag{458}$$
$$\int \langle\psi_1, \triangle F'\psi_2\rangle \, \mathrm{d}\psi_2 = \hbar^{k+1}\langle\psi_1', \psi_1\rangle \left[G_0'(\psi_1, \psi_1) + \mathcal{O}(\hbar)\right],$$
$$\int |\langle\psi_1, F\psi_2\rangle| \, \mathrm{d}\psi_2 \leq \hbar^{-3}\widetilde{\langle\psi_1', \psi_1\rangle} \left[G_0(\psi_1, \psi_1) + \mathcal{O}(\hbar)\right],$$

where the prime indicates that we do not yet have $\psi_1' = \psi_1$. Considering the overlap functions $\widetilde{\langle\psi_1', \psi_1\rangle}$ which are Gaussians with respect to the momentum, but not with respect to the position variables, we see that in our case this contains six copies of SU(2) in position space corresponding to the six adjacent edges of a vertex in the definition of the volume operator. So there are $6N$ missing Gaussians in position space having the effect that the measure ν brings in an additional negative power of $\hbar^{-3/2}$ for each missing Gaussian in position space, since each integral measure for a Gaussian in position and momentum space comes with a factor of $\hbar^{3/2}$. This means that after the integration over ψ_1 we still have an additional factor of $\hbar^{-3/2(6N)} = \hbar^{-9N}$. Moreover, each of the N factors $\widetilde{\langle\psi_1, \psi_1\rangle}$ comes according to eq. (458) with a factor of $\hbar^{-3}$. The final computable estimate for the non-computable error in eq. (454) derived in [4] is given by

$$C\, t^{(2l+1)(k+1)-12N+9}\mathrm{Pol}_{12N+10(2l+1)(k+1)}(p). \tag{459}$$

Here C is a constant of zeroth order in $\hbar$, $t = \ell_P^2/a^2 \propto \hbar$ is the dimensionless classicallity parameter with Planck length $\ell_P = \sqrt{\hbar c/G}$ for the speed of light c and gravitational constant G, the factor a is a length scale which cancels the dimension of ℓ_P and is involved in the construction of the complexifier coherent states. Furthermore, $\mathrm{Pol}_{12N+10(2l+1)(k+1)}(p)$ is a polynomial of degree $12N + 10(2l + 1)(k + 1)$ which is at least of zeroth order in $\hbar$. So in order to have a computable error estimate of order $\hbar^{k+1}$ we need at least to perform $l = l_{N,k} \geq (12N-9)/(2k+2)$ iteration steps. Some remarks: Instead of calculating an expectation value of products of Ps, $\triangle F$s and Fs like in eq. (454), we might replace some of the $\triangle F$s by $\bar{F}$s which leads to even higher orders in $\hbar$ than the one appearing in eq. (454) when estimated from above.

Notice that in semiclassical perturbation theory for LQG and AQG we have an error control, i.e. we can be sure that higher order terms become smaller and smaller so that we can obtain an estimate adapted to our need for precision.

In [3] a semiclassical limit of the extended Master constraint operator [29, 30] within AQG in a cubic topology was calculated and we will follow the procedure presented there to handle a physical Hamiltonian in section 12. It was shown in [3] that the semiclassical limit of the extended Master constraint operator reproduces the classical Master constraint expressed in the cubic topology in lowest order in $\hbar$. For this calculation the SU(2) connection and flux variables were substituted by corresponding $\mathrm{U}(1)^3$ expressions, since in the non-Abelian SU(2) case the volume operator is not diagonalizable analytically. This substitution is justified by semiclassical perturbation theory because the substitution leads to the same result in zeroth order in $\hbar$ as semiclassical perturbation theory does.

12 Generalization to Physical Hamiltonian Operators

Our aim is to calculate a semiclassical limit of the physical Hamiltonian operator derived in [5] based on the Brown-Kuchař dust model presented in [25] at least to zeroth order in $\hbar$ with methods similar to the methods developed in [3] and [4]. We choose the physical Hamiltonian based on the Brown-Kuchař dust model here because it has a functional form similar to that of the extended Master constraint which enables us to perform steps following [3]. Though, with modifications, they might also be applied to other reference matter models leading to physical Hamiltonians as discussed in section 13. For our purpose we need to generalize the methods from [3, 4] because the techniques used in [3, 4] assume a particular form of the operators that is not given for most of the physical Hamiltonian operators derived from reduced phase space models available in the literature [1, 5, 23, 26, 130]. The reason for this is that most models lead to physical Hamiltonians which contain, additionally to an inner square root, an outer square root, see also our model in part III. By this we mean that the operator corresponding to the physical Hamiltonian density is some symmetric operator and the physical Hamiltonian operator is then defined as the square root of the latter.

First we want to compare the expressions for the extended Master $\mathbf{M}$ constraint [3, 29, 30] and the physical Hamiltonian $\mathbf{H}_{\text{phys}}$ as displayed in [5]. Their classical expressions read

$$\mathbf{M} = \int_\Sigma d^3x \frac{\left[c^2 + q^{ab} c_a c_b\right]}{\sqrt{\det(q)}}(x), \tag{460}$$

$$\mathbf{H}_{\text{phys}} = \int_S d^3\sigma \sqrt{|C^2 - Q^{jk} C_j C_k|}(\sigma), \tag{461}$$

where c and c_a, $a = 1, \ldots, 3$, denote the gravitational part of the Hamiltonian constraint and diffeomorphism constraint respectively. Here Σ stands for the spatial submanifold in the foliation of a four dimensional manifold $\mathcal{M} = \mathbb{R} \times \Sigma$ and q_{ab} denotes the ADM metric, for details on this see part II. The quantities C and C_j, $j = 1, \ldots, 3$ in $\mathbf{H}_{\text{phys}}$ denote the observables associated with c and c_a in the relational formalism for the Brown-Kuchař dust model introduced in detail in [5, 25], Q^{ij} is the spatial metric observable expressed in terms of the observables associated with the Ashtekar variables and S is called the dust space (manifold) and determines the range of σ, compare part III. Notice that it is possible to include all kinds of standard matter into c, C and c_a, C_j. A difference between c, c_a and C, C_j is that while $c = c^{\text{tot}} \approx 0$ and $c_a = c_a^{\text{tot}} \approx 0$ have no additional terms which contribute to the total constraint, denoted by "tot", and weakly vanish on the constraint surface, we have $C \neq C^{\text{tot}} = C + C^{\text{dust}}$, respectively $C_j \neq C_j^{\text{tot}} = C_j + C_j^{\text{dust}}$ which then give rise to the physical Hamiltonian. The quantized AQG versions of the physical Hamiltonian constraint and the Master constraint with respect to the infinite algebraic graph γ can be found in [5].

In the following we have to keep in mind that the physical Hamiltonian $\mathbf{H}_{\text{phys}}$ contains observables, but the Master constraint $\mathbf{M}$ does not. Despite that fact, we will use the same symbols in their quantized versions because they can formally be used in a similar way, since the algebras of the elementary variables involved in $\mathbf{M}$ and $\mathbf{H}_{\text{phys}}$ are isomorphic.

Then the operators for the Master constraint and physical Hamiltonian constraint can be expressed as

$$\hat{\mathbf{M}} = \sum_{v\in V(\gamma)} \sum_{\mu=0}^{3} \hat{C}^{\dagger}_{\mu,v}\hat{C}_{\mu,v} =: \sum_{v\in V(\gamma)} \hat{\mathbf{M}}_v, \tag{462}$$

$$\hat{\mathbf{H}}_{\mathrm{phys}} = \sum_{v\in V(\gamma)} \sqrt{\left|\hat{C}^{\dagger}_{0,v}\hat{C}_{0,v} - \frac{1}{4}\hat{C}^{\dagger}_{I,v}\hat{C}_{I,v}\right|} =: \sum_{v\in V(\gamma)} \hat{\mathbf{H}}_{\mathrm{phys,v}}, \tag{463}$$

where $\sum_v$ is the sum over the vertices of the algebraic graph and we use the sum convention for $I = 1, 2, 3$.

In general the operators $\hat{C}_{\mu,v}$, sometimes denoted as $\hat{C}_{\mu,\gamma,v}$, have the following form, compare [5] eq. (3.18),

$$\begin{aligned}\hat{C}_{\mu,v} := &\frac{1}{\ell_P^2\,|T_v(\gamma)|} \sum_{(e_1,e_2,e_3)\in T_v(\gamma)} \epsilon^{IJK} \frac{1}{|L_{\gamma,v,e_I,e_J}|} \sum_{\alpha\in L_{\gamma,v,e_I,e_J}} \\ &\times \mathrm{Tr}\left(\tau_\mu \hat{h}(\alpha)\hat{h}(e_k)\left[\hat{h}(e_k)^{-1}, F(\hat{V}_{\gamma,v})\right]\right).\end{aligned} \tag{464}$$

Here $T_v(\gamma)$ stands for the set of ordered triples of distinct edges of the graph γ incident at the vertex v of γ with outgoing orientation, L_{γ,v,e_I,e_J} stands for the set of minimal loops in γ, for a definition see section 9.6.6, $\tau_\mu = -i\sigma_\mu$ with identity matrix σ_0 and Pauli matrices σ_j, $j = 1, 2, 3$ and $\hat{h}(p)$ denotes the holonomy of the connection A along a path p in γ. $F(\hat{V}_{\gamma,v})$ is an operator valued function of the volume operator $\hat{V}_{\gamma,v}$ which takes the values $F(\hat{V}_{\gamma,v}) = \hat{V}_{\gamma,v}$ for the physical Hamiltonian operator and $F(\hat{V}_{\gamma,v}) = \hat{V}^{\frac{1}{2}}_{\gamma,v}$ for the Master constraint operator.

The basic building blocks for the calculation of the expectation value of the Master constraint operator in [3] were defined as

$$\hat{O}_v := \mathrm{Tr}\left(\tau_\mu \hat{h}(\alpha)\hat{h}(e_k)\left[\hat{h}(e_k)^{-1}, F(\hat{V}_{\gamma,v})\right]\right). \tag{465}$$

With the help of this definition the Master constraint operator can be re-written as

$$\hat{\mathbf{M}} = \sum_{v\in V(\gamma)} \hat{\mathbf{M}}_v = \sum_{v\in V(\gamma)} \sum_{\mu=0}^{3} \hat{C}^{\dagger}_{\mu,v}\hat{C}_{\mu,v} \propto \sum_{v\in V(\gamma)} \left(\hat{O}_v\right)^{\dagger} \hat{O}_v, \tag{466}$$

where in [3] for the explicit computation of the semiclassical expectation value the SU(2) expressions for the holonomies and fluxes were replaced by their corresponding $\mathrm{U}(1)^3$ counterparts. Their action on the semiclassical states was calculated step by step in [3] using the results of [4] and [44, 45].

In [4] a symbolical notation for the $\hat{O}_v$ operators and similar for more general products of holonomy operators and functions of the volume operator was introduced. Using this notation $\hat{O}_v$ in eq. (465) becomes

$$p_1(\hat{h})F_1(\hat{V}_{v_1})p_2(\hat{h}) \tag{467}$$

with $F_1(\hat{V}_{v_1}) = \hat{V}^{\frac{1}{2}}_{v_1}$, i.e. $q_1 = \frac{1}{8}$ for the Master constraint operator and $F_1(\hat{V}_{v_1}) = \hat{V}_{v_1}$, i.e. $q_1 = \frac{1}{4}$ for the physical Hamiltonian constraint operator. This corresponds to the $N = 1$ case of the products in polynomials of the holonomy operators $p_j(\hat{h})$ and functions of the volume operators $F(\hat{V}_{v_i})$ in eq. (443).

Analogous to the definition above for $\hat{O}_v$ in eq. (465), we define for the calculation of the expectation value of $\hat{\mathbf{H}}_{\text{phys}}$,

$$\hat{\mathbf{h}}_{\text{phys,v}} := \hat{\mathbb{O}} := \hat{C}^{\dagger}_{0,v}\hat{C}_{0,v} - \frac{1}{4}\hat{C}^{\dagger}_{I,v}\hat{C}_{I,v}. \tag{468}$$

We will refer to this as the ***physical Hamiltonian density operator*** $\hat{\mathbf{h}}_{\text{phys,v}}$ associated with $\hat{\mathbf{H}}_{\text{phys,v}}$. Except of a relative minus sign between the $\hat{C}_{0,v}$ and $\hat{C}_{I,v}$ terms and the replacement $\hat{V}^{\frac{1}{2}}_{\alpha,v} \longrightarrow \hat{V}_{\alpha,v}$ in $\hat{C}_{\mu,v}$ the operator $\hat{\mathbf{h}}_{\text{phys,v}}$ has a quite similar structure as the Master constraint operator $\hat{\mathbf{M}}_v$. We can easily check that $\hat{\mathbf{h}}_{\text{phys,v}}$ is symmetric, however it is not obvious whether it will be positive or allows for self-adjoint extensions. Yet in the end $\hat{\mathbf{H}}_{\text{phys,v}}$ involves the absolute value of $\hat{\mathbf{h}}_{\text{phys,v}}$ and hence it is by construction a positive operator, therefore the situation for $\hat{\mathbf{H}}_{\text{phys,v}}$ is more promising as will be discussed below. The expectation value of the volume operator in the complexifier coherent states is well explored [9, 114, 115, 119, 120, 121]. For $\hat{\mathbf{h}}_{\text{phys,v}}$ or in general physical Hamiltonian (density) operators this is not the case.

12.1 Naive Semiclassical Approximation of the Outer Square Root

Let us take the difficulties concerning the expectation value of $\hat{\mathbf{h}}_{\text{phys,v}}$ in the complexifier coherent states aside for a moment and assume that we can extend semiclassical perturbation theory to this case. Under this assumption, we will now investigate how to apply semiclassical perturbation theory to the outer square root appearing in $\hat{\mathbf{H}}_{\text{phys,v}}$.

12.1.1 Preliminary Definitions

During our calculations we will use results already proven in [3, 4]. Since the operator $\hat{\mathbb{O}}$ is symmetric, we can rewrite $\hat{\mathbf{H}}_{\text{phys,v}}$ as

$$\hat{\mathbf{H}}_{\text{phys,v}} = \sqrt{\left|\hat{\mathbf{h}}_{\text{phys,v}}\right|} = \sqrt{\left|\hat{\mathbb{O}}\right|} = \left(\hat{\mathbb{O}}^2\right)^{\frac{1}{4}} = \left(\hat{\mathbb{O}}^{\dagger}\hat{\mathbb{O}}\right)^{\frac{1}{4}} \tag{469}$$

and we take the absolute of $\hat{\mathbf{h}}_{\text{phys,v}}$ to take into account possible negative values in the spectrum of $\hat{\mathbb{O}}$, compare also with the discussion in section 9.6, where it is discussed that at the classical level the expression under the square root is positive on the constraint surface.

A couple of remarks are necessary at this point: Since $\hat{\mathbf{H}}_{\text{phys,v}}$ is by construction a positive and symmetric operator, we can apply Theorem 3.1. in [140], where the self-adjointness of the (extended) Master constraint was proven. Using (iii) of Theorem 3.1. and the fact that $\hat{\mathbf{H}}_{\text{phys,v}}$ is a positive and symmetric operator for all reference matter models considered in [1, 23, 25, 28, 130] the theorem ensures that the Friedrichs extension of the symmetric operator exists. Thus, in the following we will assume $\hat{\mathbf{H}}_{\text{phys,v}}$ to be a self-adjoint operator.

In the notation of [4], which corresponds to the $N = 2$ case there and in eq. (443), $\hat{\mathbb{O}}$ contains elements of the form

$$\hat{\mathbb{O}} \propto p_1(\hat{h})F_1(\hat{V}_{v_1})p_2(\hat{h})F_2(\hat{V}_{v_2})p_3(\hat{h}). \tag{470}$$

In order to be able to use some of the results from [4], we rewrite the outer square root in $\hat{\mathbf{H}}_{\text{phys,v}}$.

Therefore, we define as a generalization of $\hat{\mathbf{H}}_{\text{phys,v}}$ an operator valued function $G(\hat{\mathbb{O}})$ by

$$G(\hat{\mathbb{O}}) := \left(\hat{\mathbb{O}}^{\dagger}\hat{\mathbb{O}}\right)^p = \langle\psi, \hat{\mathbb{O}}^2\psi\rangle^p \left(\frac{\hat{\mathbb{O}}^2}{\langle\psi, \hat{\mathbb{O}}^2\psi\rangle}\right)^p \qquad (471)$$
$$=: \langle\psi, \hat{\mathbb{O}}^2\psi\rangle^p(\hat{\mathbb{1}} + \hat{y})^p =: \langle\psi, \hat{\mathbb{O}}^2\psi\rangle^p g(\hat{y})$$

with $\hat{y} = \frac{\hat{\mathbb{O}}^2}{\langle\psi,\hat{\mathbb{O}}^2\psi\rangle} - \hat{\mathbb{1}}$ and $g(\hat{y}) = (\hat{\mathbb{1}} + \hat{y})^p$.

Here we define $G(\hat{\mathbb{O}})$ in a different way compared to $F(V_I)$ in [4] with regard to the powers p of the expectation value of $\langle\psi, \hat{\mathbb{O}}^2\psi\rangle$ because $\langle\psi, \hat{\mathbb{O}}^2\psi\rangle$ corresponds to the $N = 4$ case and the choice of the exponent p instead of $2p$ will be more convenient to use later on. [1]

The $\hat{\mathbb{O}}$ operators involve the operator valued functions $F(\hat{V}_{v_I}) = |\langle\psi, \hat{Q}_{v_I}\psi\rangle|^{2q_I} f(\hat{x}_I)$ with bounded operators $\hat{x}_I = \frac{\hat{Q}^2_{v_I}}{\langle\psi,\ Q_{v_I}\psi\rangle^2} - \hat{\mathbb{1}}$ as we explained in section 11. There we also mentioned that the expectation values $\langle\psi, f(\hat{x}_I)\psi\rangle$ are not computable analytically. Therefore, also the expectation value $\langle\psi, \hat{\mathbb{O}}^2\psi\rangle$ is not computable analytically.

To proceed with our analogy we will briefly repeat the main steps of [4] which shows that we can in principle, remembering our open questions concerning the expectation value of $\hat{\mathbf{h}}_{\text{phys,v}}$, equal to $\hat{\mathbb{O}}$, in the complexifier coherent states, expand the expectation value of $G(\hat{\mathbb{O}})$ in a series of expectation values of powers of the operator $\hat{y}$. Even though, as discussed in section 11, the application of the spectral theorem to $f(\hat{x}_I)$ in eq.(447) does not indicate that the power series expansion works and we can only apply the spectral theorem to $g(\hat{y})$, if we know that $\hat{y}$ is self-adjoint. Let us consider

$$\langle\psi, G(\hat{\mathbb{O}})\psi\rangle = \langle\psi, \hat{\mathbb{O}}^2\psi\rangle^p\langle\psi, g(\hat{y})\psi\rangle \approx \langle\hat{\mathbb{O}}^2\rangle^p\langle\psi, \left(1 + \sum_{n=1}^{\infty}\binom{p}{n}\hat{y}^n\right)\psi\rangle, \qquad (472)$$

where $|\psi\rangle$ denote the complexifier coherent states from section 18 and we used the abbreviation $\langle\hat{\mathbb{O}}^2\rangle := \langle\psi, \hat{\mathbb{O}}^2\psi\rangle$.

Here p corresponds to q in [4], see also section 11. Especially, if we set $p = \frac{1}{4}$, we will recover the physical Hamiltonian operator $\hat{\mathbf{H}}_{\text{phys}}$. For p in the range $0 < p \leq \frac{1}{4}$, we can apply Lemma 2.1. and Lemma 2.3. from [4], see appendix G. Lemma 2.1. tells us how we can estimate a function $g(t) = (1 + t)^p$ from below and above by its partial Taylor series $g_{\tilde{k}}(t)$, namely

$$g_-(t) := g_{2\tilde{k}+1}(t) - \beta_{\tilde{k}} t^{2\tilde{k}+2} \leq g(t) \leq g_{2\tilde{k}+1}(t) =: g_+(t), \qquad (473)$$

where for each $\tilde{k} \geq 0$ there exists $0 < \beta_{\tilde{k}} < \infty$ such that the estimates above hold. Lemma 2.3. gives an approximation for the non-computable expectation values $\langle\psi, g(\hat{y})\psi\rangle$ of symmetric, originally self-adjoint, operators $g(\hat{y})$ by computable ones. For this purpose we define for operators $g(\hat{y})$, $g_-(\hat{y})$, $g_+(\hat{y})$ with $g_-(\hat{y}) \leq g(\hat{y}) \leq g_+(\hat{y})$ according to Lemma 2.3.,

$$\bar{g} := \frac{(g_+ + g_-)}{2}, \quad \triangle g := \frac{(g_+ - g_-)}{4} \qquad (474)$$

[1] In a completely analogous way to [4], we could define

$$G(\hat{\mathbb{O}}) := \left(\hat{\mathbb{O}}^{\dagger}\hat{\mathbb{O}}\right)^p = \langle\psi, \hat{\mathbb{O}}\psi\rangle^{2p}\left(\frac{\hat{\mathbb{O}}^2}{\langle\psi, \hat{\mathbb{O}}\psi\rangle^2}\right)^p =: \langle\psi, \hat{\mathbb{O}}\psi\rangle^{2p}(\hat{\mathbb{1}} + \hat{y})^p,$$

with $\hat{y} = \frac{\hat{\mathbb{O}}^2}{\langle\psi,\hat{\mathbb{O}}\psi\rangle^2} - \hat{\mathbb{1}}$.

and for G

$$\bar{G} := \langle\psi, \hat{\mathbb{O}}^2\psi\rangle^p \bar{g}, \quad \triangle G := \langle\psi, \hat{\mathbb{O}}^2\psi\rangle^p \triangle g. \tag{475}$$

In this case we know from Lemma 2.3. in [4], see appendix G, that for the real part of the expectation value $\Re(\langle\psi., .\psi\rangle)$ we have the estimate

$$|\Re(\langle\psi, g(\hat{y})\psi\rangle) - \Re(\langle\psi, \bar{g}(\hat{y})\psi\rangle)| \leq 2\,\langle\psi, \triangle g(\hat{y})\psi\rangle. \tag{476}$$

The same estimate also holds for the imaginary part $\Im(\langle\psi., .\psi\rangle)$. It is important to notice that in analogy to [4], see section 11, if the expectation values of $\bar{g}$ and $\triangle g$ are computable and $|\Re(\langle\psi, [g - \bar{g}]\,(\hat{y})\psi\rangle)|$ is small, $\Re(\langle\psi, \bar{g}(\hat{y})\psi\rangle)$ will be a good approximation for $\Re(\langle\psi, g(\hat{y})\psi\rangle)$. In the following we try to determine the expectation values for $\langle\psi, \bar{g}(\hat{y})\psi\rangle$ and $\langle\psi, \triangle g(\hat{y})\psi\rangle$. In order to do so we take a closer look on their exact form and how they depend on the partial series with respect to $\tilde{k}$. To gain the expectation value for $\langle\psi, \bar{g}(\hat{y})\psi\rangle$, we use the definitions in eq. (474) which leads to the expansion

$$\begin{aligned} \langle\psi, \bar{g}(\hat{y})\psi\rangle &= \langle\psi, g_+(\hat{y})\psi\rangle - 2\,\langle\psi, \triangle g(\hat{y})\psi\rangle = \langle\psi, g_{2\tilde{k}+1}(\hat{y})\psi\rangle - \frac{\beta_{\tilde{k}}}{2}\langle\psi, \hat{y}^{2\tilde{k}+2}\psi\rangle \\ &= \sum_{n=0}^{2\tilde{k}+1}\binom{p}{n}\langle\psi, \hat{y}^n\psi\rangle - \frac{\beta_{\tilde{k}}}{2}\langle\psi, \hat{y}^{2\tilde{k}+2}\psi\rangle. \end{aligned} \tag{477}$$

From eq. (477) we see that the relevant parts in the expansion are the expectation values of $\hat{y}^n$, for $n \in \mathbb{N}_0$, in the complexifier coherent states. We will show in sections 12.1.3 and 12.1.4 that the terms containing the $\beta_{\tilde{k}}$ are always of higher order in $\hbar$ than the $\langle\psi, g_+(\hat{y})\psi\rangle$ term is. Therefore, the expectation value $\langle\psi, g_+(\hat{y})\psi\rangle$ is already a good approximation for $\langle\psi, g(\hat{y})\psi\rangle$ and we do not need to know the explicit value of the $\beta_{\tilde{k}}$ as discussed in detail in [4].

12.1.2 Basic Elements

As a consequence, our next step is to find out how the expectation values of $\hat{y}^n$ look like in dependence on the different powers of n. Also we want to relate their calculation to the approximation for the expectation value of the volume operator performed in [4]. For the trivial cases $n = 0$ and $n = 1$ we obtain $\langle\psi, \hat{y}^0\psi\rangle = 1$ and $\langle\psi, \hat{y}^1\psi\rangle = 0$. The expectation value of the operator $\hat{y}^n$ in the complexifier coherent states for general powers of n, for $n \in \mathbb{N}_0$, is given by

$$\langle\psi, \hat{y}^n\psi\rangle = \langle\psi, \left(\frac{\hat{\mathbb{O}}^2}{\langle\hat{\mathbb{O}}^2\rangle} - \hat{\mathbb{1}}\right)^n \psi\rangle = \langle\psi, \sum_{\ell=0}^{n}\binom{n}{\ell}\left(\frac{\hat{\mathbb{O}}^2}{\langle\hat{\mathbb{O}}^2\rangle}\right)^{n-\ell}(-1)^\ell\,\psi\rangle. \tag{478}$$

Because the operator difference to the power of n contains only terms of the form $\frac{\hat{\mathbb{O}}^2}{\langle\hat{\mathbb{O}}^2\rangle}$ and the unit operator $\hat{\mathbb{1}}$ which commute with each other, we can use a binomial expansion.

In the following it will also be useful to analyze how the power n of $\hat{y}$ and the number N of the F_I in the leading order term of $\hat{y}^n$ are related. As we have seen, the $\hat{y}^n$ contain powers of $\hat{\mathbb{O}}$ operators and the $\hat{\mathbb{O}}$ operators involve products of polynomials of holonomy operators p_j and functions of the volume operator F_I, see eq. (470). Hence to perform our outer estimate, we want to decompose the expectation values of $\hat{y}^n$ into "basic elements" consisting of expectation values of the $\hat{\mathbb{O}}$ operators.

To get an idea how to obtain such basic elements, we will start with the easiest $\tilde{k}=0$ case of the expansion of $\bar{g}$ in eq. (477). In the $\tilde{k}=0$ case the expectation values $\langle\psi, \triangle g(\hat{y})\psi\rangle$ and $\langle\psi, g_+(\hat{y})\psi\rangle$ become

$$\begin{aligned}\langle\psi, \triangle g(\hat{y})\psi\rangle &= \frac{\beta_0}{4}\langle\psi, \hat{y}^2\psi\rangle = \frac{\beta_0}{4}\langle\psi, \left(\frac{\hat{\mathbb{O}}^4}{\langle\hat{\mathbb{O}}^2\rangle^2} - 2\frac{\hat{\mathbb{O}}^2}{\langle\hat{\mathbb{O}}^2\rangle} + \hat{\mathbb{1}}\right)\psi\rangle \\ &= \frac{\beta_0}{4}\frac{1}{\langle\hat{\mathbb{O}}^2\rangle^2}\left(\langle\hat{\mathbb{O}}^4\rangle - \langle\hat{\mathbb{O}}^2\rangle^2\right)\end{aligned} \tag{479}$$

and

$$\langle\psi, g_+(\hat{y})\psi\rangle = \langle\psi, g_1(\hat{y})\psi\rangle = \sum_{n=0}^{1}\binom{p}{n}\langle\psi, \hat{y}^n\psi\rangle = \langle\psi, \hat{y}^0\psi\rangle + p\langle\psi, \hat{y}^1\psi\rangle = 1. \tag{480}$$

From this example we see why our definition of $\hat{y} := \frac{\hat{\mathbb{O}}^2}{\langle\psi, \hat{\mathbb{O}}^2\psi\rangle} - \hat{\mathbb{1}}$ in eq. (471) is more convenient than a completely analogous definition compared to the operator $\hat{x}_I := \frac{\hat{Q}^2_{v_I}}{\langle\psi, \hat{Q}_v\psi\rangle^2} - \hat{\mathbb{1}}$ in [4]. Here the expectation value $\langle\psi, \hat{y}^1\psi\rangle$ just vanishes. Instead of the fluctuation of $\hat{Q}$ as in [4], the corrections in the expansion involve fluctuations of the operator $\hat{\mathbb{O}}^2$. Hence, by using $\hat{y} = \frac{\hat{\mathbb{O}}^2}{\langle\psi, \hat{\mathbb{O}}^2\psi\rangle} - \hat{\mathbb{1}}$ the outer expansion gets less complicated, however the price to pay is that for the inner expansion we need to consider $\langle\hat{\mathbb{O}}^2\rangle$ corresponding to $N=4$ and not $\langle\hat{\mathbb{O}}\rangle$ corresponding to $N=2$.

The smallest non-trivial element that we can get is

$$\langle\psi, \hat{y}^2\psi\rangle = \frac{1}{\langle\hat{\mathbb{O}}^2\rangle^2}\left(\langle\hat{\mathbb{O}}^4\rangle - \langle\hat{\mathbb{O}}^2\rangle^2\right). \tag{481}$$

Since this is part of the $\beta_{\tilde{k}}$ term for $\tilde{k}=0$, we have to check, whether $\langle\psi, \hat{y}^2\psi\rangle$ is small compared to $\langle\psi, g_1(\hat{y})\psi\rangle = 1$.

12.1.3 Computation of the Smallest Non-trivial Element

This is the point were we again need to use some results from [4] regarding the inner estimate of the expectation value of the volume operator. Recall that $\langle\hat{\mathbb{O}}^2\rangle$ corresponds to the $N=4$ case of [4], i.e. it contains elements of the form

$$\begin{aligned}\langle\hat{\mathbb{O}}^2\rangle &\propto \langle p_1F_1p_2F_2p_3F_3p_4F_4p_5\rangle \\ &= \left(\prod_{I=1}^{4}|\langle\psi, \hat{Q}_{v_I}\psi\rangle|^{2q_I}\right)\langle p_1f_1p_2f_2p_3f_3p_4f_4p_5\rangle \\ &= \left(\prod_{I=1}^{4}F_{0,I}^{2q_I}\right)\langle p_1\left[1+\sum_{m_1=1}^{2k+1}\binom{q}{m_1}\hat{x}_1^{m_1}\right]p_2\left[1+\sum_{m_2=1}^{2k+1}\binom{q}{m_2}\hat{x}_2^{m_2}\right]p_3\left[1+\sum_{m_3=1}^{2k+1}\binom{q}{m_3}\hat{x}_3^{m_3}\right] \\ &\quad\times p_4\left[1+\sum_{m_4=1}^{2k+1}\binom{q}{m_4}\hat{x}_4^{m_4}\right]p_5\rangle + \mathcal{O}(\hbar^{k+1}) \\ &:= \left\langle\hat{\overline{\mathbb{O}}}^2\right\rangle + \mathcal{O}(\hbar^{k+1})\end{aligned} \tag{482}$$

and we define $F_{0,I} := |\langle \psi, \hat{Q}_{v_I} \psi \rangle|$. As explained in section 11 expectation values of this type, see also eq. (443), cannot be calculated using the spectral theorem and the power expansion shown above due to convergence issues. Though, the main result of [4] was that this power expansion approximates the non-computable expectation values reasonable well up to corrections that are of higher order in $\hbar$ than the order considered in the semiclassical perturbation theory. That is even for general $n \in \mathbb{N}_0$ we have

$$\langle \hat{\mathbb{O}}^{2n} \rangle = \left\langle \hat{\bar{\mathbb{O}}}^{2n} \right\rangle + \mathcal{O}(\hbar^{k+1}) \tag{483}$$

and thus we substituted the non-computable expectation value on the left hand side by a computable one. To achieve this, one has to apply the iteration algorithm, which was developed and proven in [4]. The errors are of higher order in $\hbar$ than the approximation $\left\langle \hat{\bar{\mathbb{O}}}^{2n} \right\rangle$ for the expectation value of the polynomials in holonomy operators and functions of the volume operator contained in $\langle \hat{\mathbb{O}}^{2n} \rangle$, provided one applies the iteration algorithm appropriately often. In other words the partial series depending on the natural number k that is used in the approximation $\left\langle \hat{\bar{\mathbb{O}}}^{2n} \right\rangle$ has to be taken up to a value of k that is large enough in order to achieve the degree of precision of the approximation that is relevant for the problem one is interested in.

The number of necessary iteration steps $\ell_{N,k}$ to obtain corrections of order $\hbar^{k+1}$ in correspondence to N and k derived in [4] is given by

$$\ell_{N,k} \geq (12N - 9)/(2k + 2). \tag{484}$$

Schematically, for the numerator $\hat{\bar{\mathbb{O}}}^{2n}$ and denominator $\left\langle \hat{\bar{\mathbb{O}}}^{2} \right\rangle^n$ in eq. (478) we have in the language of expectation values of the form $\langle \psi | p_1(\hat{h}) F_1(\hat{V}_{v_1}) \ldots p_N(\hat{h}) F_N(\hat{V}_{v_2}) p_{N+1}(\hat{h}) | \psi \rangle$, compare eq. (443), the cases:

$$\frac{N_{\text{num}} = 4 \cdot n}{(N_{\text{den}} = 4)^n}, \tag{485}$$

where N_{num} and N_{den} stand for the number of operator valued functions $F_I(\hat{V}_{v_I})$ of the volume operator involved in the numerator and denominator respectively. At this point we can use the connection between the number N of the F_I and the power n of y, given by $N = 4 \cdot n$, for the leading order term in $\langle y^n \rangle$ to find out how many iteration steps we have to perform maximally to obtain corrections of at least $\mathcal{O}(\hbar^{k+1})$. We see that we need at least

$$\ell_{4n,k} \geq (48n - 9)/(2k + 2) \tag{486}$$

steps to obtain an iteration of the desired precision.

As an example, for the $N = 4$ case, that is $n = 1$, we have

$$\ell_{4,k} \geq (48 - 9)/(2k + 2) = 39/(2k + 2). \tag{487}$$

Assume that for appropriate $\ell_{4n,k}$ and k we are able to bring $\langle \hat{\mathbb{O}}^{2n} \rangle$ into the form

$$\langle \hat{\mathbb{O}}^{2n} \rangle = \left\langle \hat{\bar{\mathbb{O}}}^{2n} \right\rangle + \mathcal{O}(\hbar^{k+1}),$$

where $\left\langle \hat{\bar{\mathbb{O}}}^{2n} \right\rangle$ is of order $\hbar^k$. In the end we want to obtain an approximation $\langle \bar{y}^2 \rangle$ for the exact expectation value $\langle y^2 \rangle$ in eq. (481). We already know, at least formally, the approximation for $\langle \hat{\mathbb{O}}^{2n} \rangle$, what is still missing is an approximation for $\frac{1}{\langle \hat{\mathbb{O}}^2 \rangle^n}$ which we expect to be of the form

$$\frac{1}{\langle \hat{\mathbb{O}}^2 \rangle^n} = \frac{1}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^n} + \mathcal{O}(\hbar^{k+1}). \tag{488}$$

To assure ourselves that our expectation for the approximation of $\frac{1}{\langle \hat{\mathbb{O}}^2 \rangle^n}$ is correct, we apply the geometric series to the expansion of $\frac{1}{\langle \hat{\mathbb{O}}^2 \rangle^n}$ which leads to

$$\begin{aligned} \frac{1}{\langle \hat{\mathbb{O}}^2 \rangle^n} &= \frac{1}{\left(\langle \hat{\bar{\mathbb{O}}}^2 \rangle + \mathcal{O}(\hbar^{k+1}) \right)^n} = \frac{1}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^n \left(1 - \left(\frac{-\mathcal{O}(\hbar^{k+1})}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle} \right) \right)^n} \\ &= \frac{1}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^n} \left(\frac{1}{1-r} \right)^n = \frac{1}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^n} \left(\sum_{b=0}^{\infty} r^b \right)^n . \end{aligned} \tag{489}$$

The last equality only holds for $|r| := \left| \frac{-\mathcal{O}(\hbar^{k+1})}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle} \right| < 1$, since otherwise, as we know from the definition of the geometric series, the series does not converge. The convergence of the series can be assured by calculating the approximation of $\langle \hat{\mathbb{O}}^2 \rangle$ up to an order in $\hbar$ that is high enough in the sense that all error terms have to be at least of one order higher in $\hbar$ than the terms inside the expansion of $\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle$. Then, the sum of terms in the denominator is larger than the sum of terms in the numerator and consequently $|r| < 1$. Finally, using eq. (488) and eq. (489) we obtain for the $\tilde{k} = 0$ case

$$\begin{aligned} \langle \psi, \triangle g(y) \psi \rangle &= \frac{\beta_0}{4} \frac{1}{\langle \hat{\mathbb{O}}^2 \rangle^2} \left(\langle \hat{\mathbb{O}}^4 \rangle - \langle \hat{\mathbb{O}}^2 \rangle^2 \right) \\ &= \frac{\beta_0}{4} \frac{1}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^2} \left(\sum_{b=0}^{\infty} r^b \right)^2 \left((\left\langle \hat{\bar{\mathbb{O}}}^4 \right\rangle + \mathcal{O}(\hbar^{k+1})) - (\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^2 + \mathcal{O}(\hbar^{k+1})) \right) \\ &= \frac{\beta_0}{4} \frac{1}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^2} \left(\sum_{b=0}^{\infty} \left(\frac{-\mathcal{O}(\hbar^{k+1})}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle} \right)^b \right)^2 \left((\left\langle \hat{\bar{\mathbb{O}}}^4 \right\rangle + \mathcal{O}(\hbar^{k+1})) - (\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^2 + \mathcal{O}(\hbar^{k+1})) \right). \end{aligned} \tag{490}$$

The dominant, i.e. largest term in the series, is the term for $b = 0$ given by

$$B_0 := \langle \psi, \triangle g(y) \psi \rangle_{b=0} = \frac{\beta_0}{4} \frac{1}{\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^2} (1 + \ldots) \left((\left\langle \hat{\bar{\mathbb{O}}}^4 \right\rangle + \mathcal{O}(\hbar^{k+1})) - (\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^2 + \mathcal{O}(\hbar^{k+1})) \right) \tag{491}$$

in lowest order in $\hbar$. This term is proportional to the fluctuations of the operator $\hat{\bar{\mathbb{O}}}^2$ rescaled by the semiclassical expectation value $\left\langle \hat{\bar{\mathbb{O}}}^2 \right\rangle^2$. To recognize of which order $\langle \psi, \triangle g \psi \rangle$ is, requires to take a closer look on the specific structure of $\left\langle \hat{\mathbb{O}}^2 \right\rangle^2$ and $\left\langle \hat{\mathbb{O}}^4 \right\rangle$. In the notation of [4], also compare eq. (443) $\left\langle \hat{\mathbb{O}}^2 \right\rangle$ is of the form

$$\begin{aligned}
\left\langle \hat{\mathbb{O}}^2 \right\rangle &:= \left(\prod_{I=1}^{4} |\langle \psi, Q_{v_I} \psi \rangle|^{2q_I} \right) \langle p_1 \bar{f}_1 p_2 \bar{f}_2 p_3 \bar{f}_3 p_4 \bar{f}_4 p_5 \rangle \qquad (492)\\
&\propto \langle p_1 \left[1 + \sum_{m_1=1}^{2k+1} \binom{q}{m_1} x_1^{m_1} \right] p_2 \left[1 + \sum_{m_2=1}^{2k+1} \binom{q}{m_2} x_2^{m_2} \right] p_3 \left[1 + \sum_{m_3=1}^{2k+1} \binom{q}{m_3} x_3^{m_3} \right] p_4 \left[1 + \sum_{m_4=1}^{2k+1} \binom{q}{m_4} x_4^{m_4} \right] p_5 \rangle \\
&\quad + \mathcal{O}(\hbar^{k+1}) \\
&\propto \langle p_1 \left[1 + \sum_{m_1=1}^{2k+1} \binom{q}{m_1} \left(\frac{Q_{v_1}^2}{\langle \psi,\ Q_{v_1} \psi \rangle^2} - \hat{\mathbb{1}} \right)^{m_1} \right] p_2 \left[1 + \sum_{m_2=1}^{2k+1} \binom{q}{m_2} \left(\frac{Q_{v_2}^2}{\langle \psi,\ Q_{v_2} \psi \rangle^2} - \hat{\mathbb{1}} \right)^{m_2} \right] \\
&\quad p_3 \left[1 + \sum_{m_3=1}^{2k+1} \binom{q}{m_3} \left(\frac{Q_{v_3}^2}{\langle \psi,\ Q_{v_3} \psi \rangle^2} - \hat{\mathbb{1}} \right)^{m_3} \right] p_4 \left[1 + \sum_{m_4=1}^{2k+1} \binom{q}{m_4} \left(\frac{Q_{v_4}^2}{\langle \psi,\ Q_{v_4} \psi \rangle^2} - \hat{\mathbb{1}} \right)^{m_4} \right] p_5 \rangle + \mathcal{O}(\hbar^{k+1}) \\
&\propto \langle p_1 \left[1 + \sum_{m_1=1}^{2k+1} \binom{q}{m_1} \frac{1}{\langle Q_{v_1} \rangle^{2m_1}} (Q_{v_1}^2 - \langle Q_{v_1} \rangle^2)^{m_1} \right] p_2 \left[1 + \sum_{m_2=1}^{2k+1} \binom{q}{m_2} \frac{1}{\langle Q_{v_2} \rangle^{2m_2}} (Q_{v_2}^2 - \langle Q_{v_2} \rangle^2)^{m_2} \right] \\
&\quad p_3 \left[1 + \sum_{m_3=1}^{2k+1} \binom{q}{m_3} \frac{1}{\langle Q_{v_3} \rangle^{2m_3}} (Q_{v_3}^2 - \langle Q_{v_3} \rangle^2)^{m_3} \right] p_4 \left[1 + \sum_{m_4=1}^{2k+1} \binom{q}{m_4} \frac{1}{\langle Q_{v_4} \rangle^{2m_4}} (Q_{v_4}^2 - \langle Q_{v_4} \rangle^2)^{m_4} \right] p_5 \rangle \\
&\quad + \mathcal{O}(\hbar^{k+1}),
\end{aligned}$$

where we used that $\bar{f} = f_+ + \mathcal{O}(\hbar^{k+1})$. For clarity and completeness we also recall here that $\langle \hat{\mathbb{O}}^4 \rangle$ corresponds to the $N = 8$ case of [4] or eq. (443) with repeating indices, i.e.

$$\begin{aligned}
\langle \hat{\mathbb{O}}^4 \rangle &\propto \langle p_1 F_1 p_2 F_2 p_3 F_3 p_4 F_4 p_5 p_1 F_1 p_2 F_2 p_3 F_3 p_4 F_4 p_5 \rangle \qquad (493)\\
&= \left(\prod_{I=1}^{4} |\langle \psi, Q_{v_I} \psi \rangle|^{2q_I} \right)^2 \langle p_1 [1 + f_1] p_2 [1 + f_2] p_3 [1 + f_3] p_4 [1 + f_4] p_5 \\
&\quad \times p_1 [1 + f_1] p_2 [1 + f_2] p_3 [1 + f_3] p_4 [1 + f_4] p_5 \rangle.
\end{aligned}$$

With the help of this expression it will be easy to calculate the expectation value for the estimate of $\left\langle \hat{\mathbb{O}}^4 \right\rangle$. Notice that the prefactors of $\left\langle \hat{\mathbb{O}}^2 \right\rangle^2$ and $\left\langle \hat{\mathbb{O}}^4 \right\rangle$ in the enumerator and denominator in eq. (491) cancel against each other because the indices $I = 1, 2, 3, 4$ repeat themselves, that is $\prod_{I=1}^{8} |\langle \psi, Q_{v_I} \psi \rangle|^{2q_I} = (\prod_{I=1}^{4} |\langle \psi, Q_{v_I} \psi \rangle|^{2q_I})^2$.

Now we consider the $\mathcal{O}(1)$ terms containing only the holonomy operators

$$\begin{aligned}
\left\langle \hat{\mathbb{O}}^2 \right\rangle^2 &\propto (\langle \hat{p}_1 \hat{p}_2 \hat{p}_3 \hat{p}_4 \hat{p}_5 \rangle)^2 + \dots \qquad (494)\\
\left\langle \hat{\mathbb{O}}^4 \right\rangle &\propto \langle \hat{p}_1 \hat{p}_2 \hat{p}_3 \hat{p}_4 \hat{p}_5 \hat{p}_1 \hat{p}_2 \hat{p}_3 \hat{p}_4 \hat{p}_5 \rangle + \dots .
\end{aligned}$$

Here we display the operators with a hat, i.e. $\hat{p}_j$, to make it easier to distinguish them from the classical values of the polynomials in the holonomies p_j. Applying Theorem 3.3 in [45], eq. (3.127), we find

$$\left(\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle_g^t\right)^2 \propto (p_1(g)p_2(g)p_3(g)p_4(g)p_5(g)[1+\mathcal{O}(\hbar)])^2 \tag{495}$$
$$= p_1(g)p_2(g)p_3(g)p_4(g)p_5(g)p_1(g)p_2(g)p_3(g)p_4(g)p_5(g)[1+\mathcal{O}(\hbar)]+\ldots$$
$$\left\langle\hat{\bar{\mathbb{O}}}^4\right\rangle_g^t \propto p_1(g)p_2(g)p_3(g)p_4(g)p_5(g)p_1(g)p_2(g)p_3(g)p_4(g)p_5(g)[1+\mathcal{O}(\hbar)]\ldots.$$

The coherent states $\psi = \psi_g^t$ on the left hand side of the equation are actually labeled by classical points in the phase space g, on which the holonomies are evaluated, for details see section 18. So up to higher order corrections in $\hbar$ the expectation values of products of holonomy operators yield to the products of classical holonomies. Furthermore, Theorem 3.6 and Corollary 3.1 in [44] tell us that to leading order in $\hbar$, which is $\mathcal{O}(1)$, also the expectation values of expressions of the mixed type of holonomy operators and $\bar{f}$ or only products of $\bar{f}$, that is

$$\langle\hat{p}_1\hat{\bar{f}}_1\hat{p}_l\cdots\hat{\bar{f}}_c\rangle_g^t = p_1(g)\bar{f}_1(g)p_l(g)\cdots\bar{f}_c(g)+\mathcal{O}(\hbar) \tag{496}$$

reproduce the classical values depending on the phase space point g, since the Q_v contained in $\bar{f}_i$'s are polynomials of the electric flux operators. The index c just denotes an arbitrary place holder for a natural number depending on how many $\bar{f}_i$'s are contained in the product of interest. For this reason the $\mathcal{O}(1)$ terms of $\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle^2$ and $\left\langle\hat{\bar{\mathbb{O}}}^4\right\rangle$ cancel.

The detailed investigation, given above, of the $\mathcal{O}(1)$ terms leads to the conclusion that they cancel out and we are left with contributions at least of first order in $\hbar$, that is

$$B_0 = \frac{\beta_0}{4}\mathcal{O}(1)\left(\mathcal{O}(\hbar)+\ldots+\mathcal{O}(\hbar^{k+1})-[\mathcal{O}(\hbar)+\ldots+\mathcal{O}(\hbar^{k+1})]\right). \tag{497}$$

One more subtlety, to make sure that B_0 is small compared to one, we further have to assume that the terms occurring in $\mathcal{O}(\hbar)$ next to the $\hbar$-terms themselves do not become arbitrarily large compared to $\hbar$. However, except from the scaling with $\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle^2$, these are exactly the fluctuations of the $\hat{\bar{\mathbb{O}}}^2$ operator. So we assume that the fluctuations of $\hat{\bar{\mathbb{O}}}^2$ are small. Under this assumption, we can say that $\langle\psi, y^2\psi\rangle$ is indeed small compared to $\langle\psi, g_1\psi\rangle = 1$ as demanded in eq. (477) for the $\tilde{k}=0$ case. Thus, in the $\tilde{k}=0$ case $\Re(\langle\psi, g_1\psi\rangle) = \Re(\langle\psi, g_+\psi\rangle) = 1$ is a good approximation for $\Re(\langle\psi, g\psi\rangle)$ and we can drop the term containing β_0, since it is at least of $\mathcal{O}(\hbar)$.Taking this into consideration, we conclude that also for $\tilde{k}>0$ the terms including $\beta_{\tilde{k}}$ will always be smaller or contain higher powers of $\hbar$ than the $\Re(\langle\psi, g_+\psi\rangle)$ terms, compare eq. (477), so we do not need to determine the explicit values for $\beta_{\tilde{k}}$ to obtain a defined approximation for $\Re(\langle\psi, g\psi\rangle)$.

Our approximation $\langle\bar{y}^2\rangle$ for $\langle y^2\rangle$ to leading order in $\hbar$ is therefore simply given by

$$\langle\psi, \bar{y}^2\psi\rangle = \frac{1}{\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle^2}\left(\left\langle\hat{\bar{\mathbb{O}}}^4\right\rangle - \left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle^2\right)+\mathcal{O}(\hbar^{k+1}). \tag{498}$$

In contrast to [4] we also need to approximate the prefactors $\langle\hat{\mathbb{O}}^2\rangle^p$ to obtain $G(\hat{\mathbb{O}})$, since they are not computable analytically. Their approximation in terms of computable expressions is then just given by

$$\langle\hat{\mathbb{O}}^2\rangle^p = \left(\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle+\mathcal{O}(\hbar^{k+1})\right)^p. \tag{499}$$

In summary to leading order in $\hbar$ we obtain for $\langle\psi, G(\hat{\mathbb{O}})\psi\rangle$

$$\begin{aligned}\langle G(\hat{\mathbb{O}})\rangle &= \langle\hat{\mathbb{O}}^2\rangle^p\langle g(y)\rangle = \langle\hat{\mathbb{O}}^2\rangle^p\langle\left(1+\sum_{n=1}^{\infty}\binom{p}{n}y^n\right)\rangle, = \langle\hat{\mathbb{O}}^2\rangle^p\langle g_+(y)\rangle + \mathcal{O}(\hbar^{k+1}) \\ &\stackrel{k=0}{=} \left(\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle + \mathcal{O}(\hbar)\right)^p \times (1+\mathcal{O}(\hbar)) = \left(\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle\right)^p + \mathcal{O}(\hbar).\end{aligned} \tag{500}$$

Therefore, for $p = \frac{1}{4}$ and for the terms of lowest order in $\hbar$ we have

$$\langle\hat{\mathbf{H}}_{\text{phys,v}}\rangle = \left(\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle\right)^{\frac{1}{4}} + \mathcal{O}(\hbar), \tag{501}$$

where again we assume that the fluctuations of $\hat{\bar{\mathbb{O}}}^2$ are small. So we see that to zero order in $\hbar$ instead of calculating the expectation value of the root of the operator $\hat{\mathbb{O}}^2$ we can first calculate the expectation value of $\hat{\mathbb{O}}^2$ using the approximation of [4] and then take the square root out of it. To handle the $\tilde{k} > 0$ cases we can proceed in a similar way.

12.1.4 General Case

For the general case $\tilde{k} > 0$ we will not perform a detailed analysis, however we want to point out some features for arbitrary $\tilde{k}$ which are relevant when operators with an outer and inner square root or more general fractional power are considered. As before, we mainly focus on the $\mathcal{O}(1)$ case which corresponds to the classical limit and assume that the fluctuations of $\hat{\bar{\mathbb{O}}}^2$ are small.

Remember that $\langle\psi, \bar{g}(y)\psi\rangle = \langle\psi, g_+(y)\psi\rangle - 2\langle\psi, \triangle g(y)\psi\rangle$ for general $\tilde{k}$ the expectation values $\langle\psi, g_+(y)\psi\rangle$ and $2\langle\psi, \triangle g(y)\psi\rangle$ look like

$$\begin{aligned}\langle\psi, g_+(y)\psi\rangle &= \sum_{n=0}^{2\tilde{k}+1}\binom{p}{n}\langle\psi, y^n\psi\rangle = \langle\psi, y^0\psi\rangle + p\langle\psi, y^1\psi\rangle + \sum_{n=2}^{2\tilde{k}+1}\binom{p}{n}\langle\psi, y^n\psi\rangle \\ &= 1 + \sum_{n=2}^{2\tilde{k}}\binom{p}{n}\langle\psi, y^n\psi\rangle + \binom{p}{2\tilde{k}+1}\langle\psi, y^{2\tilde{k}+1}\psi\rangle\end{aligned} \tag{502}$$

and

$$\begin{aligned}2\langle\psi, \triangle g(y)\psi\rangle &= \frac{\beta_{\tilde{k}}}{2}\langle\psi, y^{2\tilde{k}+2}\psi\rangle = \frac{\beta_{\tilde{k}}}{2}\langle\psi, \left(\frac{\hat{\mathbb{O}}^{2(2\tilde{k}+2)}}{\langle\hat{\mathbb{O}}^2\rangle^{2\tilde{k}+2}} \pm \ldots \pm \hat{\mathbb{1}}\right)\psi\rangle \\ &= \frac{\beta_{\tilde{k}}}{2}\frac{1}{\langle\hat{\mathbb{O}}^2\rangle^{2\tilde{k}+2}}\left(\langle\hat{\mathbb{O}}^{2(2\tilde{k}+2)}\rangle \pm \ldots \pm \langle\hat{\mathbb{O}}^2\rangle^{2\tilde{k}+2}\right)\end{aligned} \tag{503}$$

So the $\mathcal{O}(1)$ terms for arbitrary $\tilde{k}$ read

$$\begin{aligned}\left\langle\hat{\bar{\mathbb{O}}}^2\right\rangle^{2\tilde{k}+2} &\hat{=} \langle N=4\rangle^{2\tilde{k}+2} \hat{=} \left(\langle N=4\rangle^2\right)^{\tilde{k}+1} \\ &\propto \left((p_1(g)p_2(g)p_3(g)p_4(g)p_5(g) + p_1(g)\bar{f}_1(g)p_l(g)\cdots\bar{f}_c(g))[1+\mathcal{O}(\hbar)]\right)^{2\tilde{k}+2} \\ &= ((p_1(g)p_2(g)p_3(g)p_4(g)p_5(g)p_1(g)p_2(g)p_3(g)p_4(g)p_5(g) \\ &+ \ldots + p_1(g)\bar{f}_1(g)p_l(g)\cdots\bar{f}_c(g)p_1(g)\bar{f}_1(g)p_l(g)\cdots\bar{f}_c(g))[1+\mathcal{O}(\hbar)])^{\tilde{k}+1}\end{aligned} \tag{504}$$

and

$$\left\langle \hat{\mathbb{O}}^{2(2\tilde{k}+2)} \right\rangle \hat{=} \langle N = 4(2\tilde{k}+2)\rangle \hat{=} \langle N = 8(\tilde{k}+1)\rangle \tag{505}$$
$$\propto ((p_1(g)p_2(g)p_3(g)p_4(g)p_5(g)p_1(g)p_2(g)p_3(g)p_4(g)p_5(g)$$
$$+ \ldots + p_1(g)\bar{f}_1(g)p_l(g)\cdots\bar{f}_c(g)p_1(g)\bar{f}_1(g)p_l(g)\cdots\bar{f}_c(g))[1+\mathcal{O}(\hbar)])^{\tilde{k}+1}.$$

Hence the $\mathcal{O}(1)$ terms of $\left\langle \hat{\mathbb{O}}^2 \right\rangle^{2\tilde{k}+2}$ and $\left\langle \hat{\mathbb{O}}^{2(2\tilde{k}+2)} \right\rangle$ for arbitrary $\tilde{k}$ cancel in general. Their prefactors in the enumerator and denominator in eq. (503), like in the $\tilde{k}=0$ case, cancel against each other .

The number of iteration steps for $\hat{\mathbb{O}}^{2(2\tilde{k}+2)} \hat{=} \left(N = 4(2\tilde{k}+1)\right)$ is given by

$$\ell_{4(2\tilde{k}+1),k} \geq (48(2\tilde{k}+1)-9)/(2k+2) = (96\tilde{k}+39)/(2k+2) \tag{506}$$

and analogous for $\hat{\mathbb{O}}^{2(2\tilde{k}+2)} \hat{=} \left(N = 4(2\tilde{k}+2)\right)$ we have

$$\ell_{4(2\tilde{k}+2),k} \geq (48(2\tilde{k}+2)-9)/(2k+2) = (96\tilde{k}+87)/(2k+2) \tag{507}$$

The structure of the result is

$$\langle G(\hat{\mathbb{O}})\rangle = \left\langle \hat{\mathbb{O}}^2 \right\rangle^p \left(1 + C_p \frac{\left\langle \hat{\mathbb{O}}^4 \right\rangle - \left\langle \hat{\mathbb{O}}^2 \right\rangle^2}{\left\langle \hat{\mathbb{O}}^2 \right\rangle^2} + \ldots\right), \tag{508}$$

in each of the $\left\langle \hat{\mathbb{O}}^2 \right\rangle$, $\left\langle \hat{\mathbb{O}}^4 \right\rangle$, ... inner power series expansion with $\mathcal{O}(1)$, $\mathcal{O}(\hbar)$ ... etc. terms and C_p denotes a prefactor. Due to the one in the bracket above and the one that is involved in the inner expansion of $\left\langle \hat{\mathbb{O}}^2 \right\rangle^p$, we need to expand the inner and outer series up to the same order as we otherwise will miss $\mathcal{O}(\hbar)$ contributions. The same applies to any other choosen order of k. These considerations give us the general rule: to obtain $\mathcal{O}(\hbar^k)$ terms in the combined approximation we need to have $\tilde{k} = k$.

13 Conclusions

We explored the possibility to extend semiclassical perturbation theory within Loop or Algebraic Quantum Gravity to the class of physical Hamiltonian operators, where we explicitly displayed how the approximation works for the case of the Brown-Kuchař dust model. We described schematically how the calculation for the zeroth order in $\hbar$, which is the $\tilde{k}=0$ case of the approximation, works and shortly discussed some features for higher orders in $\hbar$. In order to analyze this, two assumptions play a pivotal role: the first one is that the physical Hamiltonian operator is a self-adjoint operator which was discussed to be given, since it is implemented as a positive and symmetric operator in the physical Hilbert space. The second assumption is that the fluctuations of $\hat{\mathbb{O}}^2$ are sufficiently small such that the power series expansion of the outer square root is satisfied. This was not analyzed in detail here and goes beyond the scope of this thesis. Note that if we had defined $\hat{y} := \frac{\hat{\mathbb{O}}^2}{\langle\psi,\hat{\mathbb{O}}\psi\rangle^2} - \hat{\mathbb{1}}$, then the requirement would have carried over to the fluctuations of $\hat{\hat{\mathbb{O}}}$ instead. In general we expect that the fluctuations grow with an increasing power of the operator. However, since we did not analyze those fluctuations in detail here but just elaborated the general scheme, we choose the definition of $\hat{y}$ such that the outer expansion simplifies.

It was shown that to zeroth order in $\hbar$ instead of calculating the expectation value of the square root appearing in the physical Hamiltonian operator $\hat{\mathbf{H}}_{\mathrm{phys,v}}$ of the Brown-Kuchař dust model, we can also approximate the expectation value of the physical Hamiltonian density operator $\hat{\mathbf{h}}_{\mathrm{phys,v}}$ in complexifier coherent states and take the square root afterwards. The biggest obstacle in this approximation is that we tried to rewrite the occurring expressions in terms of expectation values of the form $\langle\psi, \hat{\mathbb{O}}^2\psi\rangle$, where $\hat{\mathbb{O}} = \hat{\mathbf{h}}_{\mathrm{phys,v}}$ whose expectation value in the complexifier coherent states is unknown. However, we know that $\hat{\mathbb{O}}$ contains elements of the form $p_1(\hat{h})F_1(\hat{V}_{v_1})p_2(\hat{h})F_2(\hat{V}_{v_2})p_3(\hat{h})$ whose expectation values for $0 < q \leq \frac{1}{4}$ can be approximated by computable elements by the methods of [4]. In case of the Brown-Kuchař dust model we have $q = \frac{1}{4}$, so we used that we can in principle approximate these elements with an inner power series expansion. The circumstance that we first needed to approximate $\langle\psi, \hat{\mathbb{O}}^2\psi\rangle$ which are also building blocks of our approximation for the expectation value of $\hat{\mathbf{H}}_{\mathrm{phys,v}}$ itself leads to several interlaced and dependent approximations. Despite that we explicitly investigated the Brown-Kuchař dust model the techniques introduced here can also be applied to other models if they satisfy the assumptions, which is related to the exact structure of products of holonomy and flux operators in the physical Hamiltonian operator in consideration. Since the power series expansion, depending on the chosen definition of the $\hat{y}$ operator, always involves fluctuations of the same power of the physical Hamiltonian operator in consideration, for each model it must be checked, whether the fluctuations are small.
Another point is that here the coherent states were chosen before the fractional operator was substituted by a power series of operators yielding to corrections which one will obtain, if one applies the fractional power to the expectation value. To compute this correction particularly for the case of the inner and outer fractional powers, although in principle possible with these techniques, can easily become complicated, especially for higher orders in $\hbar$. This motivates us instead of applying semiclassical perturbation theory to physical Hamiltonian operators to search for semiclassical states which are better adapted to our task of calculating the semiclassical limit of physical Hamiltonian operators including an outer square root.

Co-Authorship Declaration for Part V

Contribution of Almut Vetter to the publication: "Coherent states for fractional powers of the harmonic oscillator Hamiltonian"
preprint, arXiv:2109.06104 (gr-qc)

As a co-author I confirm that Almut Vetter contributed significantly to the results of the publication "Coherent states for fractional powers of the harmonic oscillator Hamiltonian". This involves her work on the conceptual questions, the technical methods as well as the content of this article. In particular this involves all calculations on the AQG-algorithm displayed in the article, on coherent states for constrained systems as well as developing ideas and strategies how to modify the coherent state construction for fractional powers of the harmonic oscillator Hamiltonian. The presentation of the work in the thesis summarises well her contributions to the publication.

Kristina Giesel

Kristina Giesel

Part V
Semiclassical and Coherent States

Large parts of section 22 and section 23 are contained in the article [71].

14 Motivation and Basic Problems

During the construction of physical Hamiltonian operators, except from the Gaussian dust case, we arrive at Hamiltonians classically or Hamiltonian operators at the quantum level which contain at least one outer square root, see parts III, IV and for example [23]. In part IV we derived an enlarged semiclassical perturbation framework that allows us under certain assumptions to approximate the expectation values of the square root Hamiltonian operators in the standard complexifier coherent states constructed in [43, 44, 45] and displayed in section 18. Since higher order calculations are getting quite involved, one could ask the question whether there exist semiclassical (coherent) states which are better adapted to the square root Hamiltonian operators. To make things more easy, here we consider different types of quantum mechanical toy models, i.e. with finite degrees of freedom, and no QFT or even LQG models. As we will see in this part there are some methods to handle our square root Hamiltonian operator toy models. Our special toy model will be the square root or more general a fractional power of the harmonic oscillator Hamiltonian (operator) which we simply call ***square root*** or ***fractional Hamiltonian*** (operator). The square root Hamiltonians are rather unusual in the formulation of the standard quantum mechanical framework where time is usually given as an external non-dynamical parameter. It will turn out that most of the methods to construct semiclassical or coherent states are connected to the question whether we are able to find a suitable representation, i.e. operator algebra, of the underlying physical problem. In summary we considered the following problems and possible methods to understand more in detail how the construction of semiclassical states is adapted to the dynamics of a physical system:

- Problem: Square Root Hamiltonian (operator):
  Inverse Thiemann Identity, Phase Operators and Phase States, Klauder Coherent States, Kumei method, Physical Coherent States for Constrained Systems, Coherent States for Fractional Poisson Distributions
- Problem: $H = \frac{p^2}{2m} + V(q)$, general potentials $V(q) \neq 0$ in q, especially polynomials in q:
  Complexifier Coherent States, Stephani, Dothan, Kumei method, SUSY potentials (appendix H)

We will treat all of the different methods at length in the course of this part and some in the appendix H. The idea that a quantum system should reproduce the classical system for high energies goes back to Bohr [141] and was established by Schrödinger by the construction of the coherent states for the harmonic oscillator [142]. We will start with an overview of the defining properties of semiclassical and coherent states. Next, as an introduction to the construction of semiclassical (coherent) states, we will recall the problem of the harmonic oscillator which is the first physical problem coherent states were introduced for by Schrödinger in [142] and which is still the source of inspiration for the development of methods to construct coherent states for general physical problems. After this we will display the different methods to construct semiclassical or coherent states we dealt with. The methods can be characterized with the help of two main ideas which basically describe the same by using the algebra corresponding to the physical system but number one starts from a physical and number two from a mathematical point of view:

1. Start with physical considerations to construct annihilation and creation operators $\hat{A}_i$ and $\hat{A}_i^\dagger$ such that the Hamiltonian operator factorizes as $\hat{H} = \hat{A}_i^\dagger \hat{A}_i$. Then consider the algebra generated by $\hat{H}$, $\hat{A}_i$, $\hat{A}_i^\dagger$ and the corresponding unit element $\hat{\mathbb{1}}$. Try to find an eigenstate of the generalized annihilation operator. The resulting state might serves as a semiclassical state depending on how information about the classical trajectory is implemented in its labels.

2. Start with a (Lie) algebra which takes the symmetries of the physical system into account. Take an exponential of the algebra elements containing labels which are related to the classical system and apply it to a cyclic vector of the underlying Hilbert space to obtain a semiclassical state.

14.1 Definitions Semiclassical and Coherent States

In the following we will closely stick to the presentation given in [9, 31], but will make some additions motivated by other authors [32, 33, 34].

Semiclassical states ψ_m are quantum states, that is they are elements of a Hilbert space $\mathcal{H}$, but they are related or labeled by classical points m in the phase space $\mathcal{M}$. Their defining property is that the expectation value of a quantum operator $\langle\psi_m, \hat{O}\psi_m\rangle$ reproduces at least approximately, up to small "quantum corrections", the behaviour of the related classical phase space function $O(m)$. This is expressed by the conditions:

1. Expectation Value Property:

$$\left|\frac{\langle\psi_m, \hat{O}\psi_m\rangle}{O(m)} - 1\right| \ll 1. \tag{509}$$

   Implies peakedness of the expectation value of the quantum operator around the classical value.

2. Ehrenfest Property:

$$\left|\frac{\langle\psi_m, \left[\hat{O}, \hat{O}'\right]\psi_m\rangle}{i\hbar\{O(m), O'(m)\}} - 1\right| \ll 1. \tag{510}$$

   Means that the expectation value of the commutator of the quantum operator reassembles the Poisson bracket.

3. Fluctuation Property:

$$\left|\frac{\langle\psi_m, \hat{O}^2\psi_m\rangle}{\langle\psi_m, \hat{O}\psi_m\rangle^2} - 1\right| \ll 1. \tag{511}$$

   Implies that the "quantum corrections" are small.

It is important to notice that states which behave semiclassically for one operator $\hat{O}$ do not need to behave semiclassically for a different operator $\hat{O}'$. Hence, whether a state is a semiclassical state or not depends on the operator in consideration. In the upcoming sections we will see that the functional form of the operator, we want to construct semiclassical states for, should be reflected by the construction method for the semiclassical states. By this we mean that the construction of the semiclassical states is adapted to the dynamics of the physical system.

Semiclassical states do not need to be coherent states, however coherent states often have semiclassical properties like reproducing the classical phase space function at least approximately when the expectation value of the operator in the corresponding state is taken. Despite that, people like in general to work with coherent states as semiclassical states, since they have some nice additional mathematical properties. A property which all coherent states share is:

4. Overcompleteness (Resolution of Identity):

$$\hat{\mathbb{1}}_{\mathcal{H}} = \int\limits_{\mathcal{M}} \mathrm{d}\nu(m) |\psi_m\rangle\langle\psi_m| \tag{512}$$

   for a measure ν on $\mathcal{M}$.

The following properties are not demanded to be satisfied by all authors for all types of generalized coherent states, see for example [32, 33, 34]:

5. Eigenstate of an Annihilation Operator: Given an annihilation operator $\hat{A}$, we construct eigenstates for $\hat{A}$ such that

$$\hat{A}|\psi_m\rangle = \alpha|\psi_m\rangle \tag{513}$$

   for $\alpha \in \mathbb{C}$.

6. Minimal Uncertainty Relation: For self-adjoint operators $\hat{q} = C_q \left(\hat{A} + \hat{A}^\dagger\right)/2$ and $\hat{p} = C_p \left(\hat{A} - \hat{A}^\dagger\right)/2i$ with real constants C_q, C_p and $\langle . \rangle_m = \langle \psi_m, . \psi_m \rangle$ the Heisenberg uncertainty relation is saturated, that is

$$\langle \left(\hat{q} - \langle \hat{q}^2 \rangle_m\right)^2 \rangle_m = \langle \left(\hat{p} - \langle \hat{p}^2 \rangle_m\right)^2 \rangle_m = \frac{\hbar}{2} |\langle [\hat{q}, \hat{p}] \rangle_m|. \tag{514}$$

7. Displacement Operator Property: There exist operators $\hat{G}_i$, i element of an index set, as generators of a quantum algebra such that ψ_m is created by

$$|\psi_m\rangle = e^{\sum_i \alpha_i \hat{G}_i} |\Omega\rangle, \tag{515}$$

   where $|\Omega\rangle$ is a cyclic vector of the Hilbert space, usually a vacuum state, $\alpha_i \in \mathbb{C}$ and α_i or the eigenvalues of the $\hat{G}_i$ are related to the classical phase space point m.

8. Peakedness Property: For any m, $m' \in \mathcal{M}$, the overlap function

$$m' \mapsto |\langle \psi_m, \psi_{m'} \rangle|^2 \tag{516}$$

   is concentrated in a phase cell of Liouville volume $\frac{1}{2}|\langle [\hat{q}, \hat{p}] \rangle_m|$ if $\hat{q}$ is a position and $\hat{p}$ is a momentum operator.

14.2 Review Time-independent Harmonic Oscillator

Since the harmonic oscillator is the first system coherent states were constructed for and their construction principles are generalized later on, we will summarize and review some properties of the standard time-independent harmonic oscillator and its coherent states, see for example [35, 36, 37, 38]. The classical Hamiltonian for the ***one-dimensional time-independent harmonic oscillator*** has the form

$$H_{\mathrm{ho}} = \frac{1}{2m}p^2 + \frac{1}{2}m\omega_0^2 q^2, \tag{517}$$

where q and p are the canonically conjugate phase space variables for position and momentum, that is they satisfy the Poisson brackets $\{q,p\} = 1$ and $\{q,q\} = \{p,p\} = 0$, here m is the mass of the oscillator and ω_0 denotes the time-independent frequency. The classical equations of motion have the following solutions for the position q and momentum p

$$\begin{aligned} q(t) &= A_1\cos(\omega_0 t) + A_2\sin(\omega_0 t) = A_0\cos(\omega_0 t + \delta), \\ p(t) &= B_1\cos(\omega_0 t) + B_2\sin(\omega_0 t) = B_0\sin(\omega_0 t + \delta), \end{aligned} \tag{518}$$

with constants $A_I, B_I \in \mathbb{R}$, $I = 0,1,2$, $\forall t \in \mathbb{R}^+$ and δ is a phase. For more than one one-dimensional harmonic oscillator, the Hamiltonian becomes

$$H_{\mathrm{ho}} = \sum_{i=1}^{N} \frac{1}{2m}p_i^2 + \frac{1}{2}m{\omega_0}_i^2 q_i^2, \tag{519}$$

where now the index i denotes each single oscillator and we have $\{q_i, p_j\} = \delta^i_j$ and $\{q_i, q_j\} = \{p_i, p_j\} = 0$.

The time-independent harmonic oscillator can be quantized using the so-called ***Schrödinger representation*** for q and p. Then the Hamilton operator is given by

$$\hat{H}_{\mathrm{ho}} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0^2\hat{q}^2. \tag{520}$$

Here $\hat{q}$ and $\hat{p}$ are the self-adjoint position and momentum operators and they satisfy the commutation relations

$$[\hat{q},\hat{p}] = i\hbar\hat{\mathbb{1}}, \quad [\hat{p},\hat{p}] = [\hat{q},\hat{q}] = 0. \tag{521}$$

Schrödinger was confronted with the problem how to relate the solutions of the Schrödinger equation of the time-independent harmonic oscillator with the classical solutions. This is why the concept of coherent states was introduced in [142].

Let us rewrite the Hamiltonian operator in terms of the so-called (bosonic) creation and annihilation operators. For this reason we define the ***annihilation operator*** by

$$\hat{a} := \sqrt{\frac{m\omega_0}{2\hbar}}\hat{q} + i\frac{1}{\sqrt{2\hbar m\omega_0}}\hat{p} \tag{522}$$

and the to $\hat{a}$ adjoint ***creation operator*** by

$$\hat{a}^\dagger := \sqrt{\frac{m\omega_0}{2\hbar}}\hat{q} - i\frac{1}{\sqrt{2\hbar m\omega_0}}\hat{p}. \tag{523}$$

In case that we substitute $\hat{q}$ and $\hat{p}$ by $\hat{a}$ and $\hat{a}^\dagger$, the Hamiltonian operator becomes

$$\hat{H}_{\mathrm{ho}} = \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\hat{\mathbb{1}} \right), \tag{524}$$

with the ***Weyl-Heisenberg algebra***

$$\left[\hat{a}, \hat{a}^\dagger\right] = \hat{\mathbb{1}}, \quad \left[\hat{a}^\dagger, \hat{a}^\dagger\right] = [\hat{a}, \hat{a}] = 0. \tag{525}$$

We define the ***number operator*** $\hat{n} := \hat{a}^\dagger \hat{a}$ with eigenstates $|n\rangle$ such that

$$\hat{n}|n\rangle = n|n\rangle, \tag{526}$$

with $n \in \mathbb{N}_0$. It counts the number of generated quanta. The annihilation and creation operators act on the $|n\rangle$ in the following way

$$\begin{aligned} \hat{a}|n\rangle &= \sqrt{n}|n-1\rangle, \\ \hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle. \end{aligned} \tag{527}$$

The spectrum of the time-independent harmonic oscillator is equally spaced and bounded from below. Its ***ground state*** is denoted by $|0\rangle$ and satisfies $\hat{a}|0\rangle = 0$. With this follows that every number operator eigenstate can be obtained by repeated application of the annihilation operator to the ground state $|0\rangle$, namely

$$|n\rangle = \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}}|0\rangle. \tag{528}$$

The ***coherent states for the time-independent harmonic oscillator*** or at a fixed time $t = t_0$ are given by

$$|\alpha\rangle = \exp(-\frac{1}{2}|\alpha|^2) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{529}$$

for $\alpha \in \mathbb{Z}$. They can be defined and obtained in three ways:

1. Eigenstates of the Annihilation Operator $\hat{a}$:
As one can easily check the $|\alpha\rangle$ satisfy

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \tag{530}$$

which can also be used as a defining property.

2. Displacement Operator Coherent States:
We define the unitary ***displacement operator*** $D(\alpha)$ by

$$D(\alpha) := \exp(\alpha\hat{a}^\dagger - \alpha^*\hat{a}) = \exp(-\frac{1}{2}|\alpha|^2)\exp(\alpha\hat{a}^\dagger)\exp(-\alpha^*\hat{a}) \tag{531}$$

for $\alpha \in \mathbb{Z}$ and apply it to the ground state $|0\rangle$, explicitly

$$\begin{aligned} D(\alpha)|0\rangle &= \exp(-\frac{1}{2}|\alpha|^2)\exp(\alpha\hat{a}^\dagger)\exp(-\alpha^*\hat{a})|0\rangle = \exp(-\frac{1}{2}|\alpha|^2)\exp(\alpha\hat{a}^\dagger)|0\rangle \\ &= \exp(-\frac{1}{2}|\alpha|^2)\sum_n \frac{(\alpha\hat{a}^\dagger)^n}{n!}|0\rangle = \exp(-\frac{1}{2}|\alpha|^2)\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle = |\alpha\rangle. \end{aligned} \tag{532}$$

The displacement operator can also be used to obtain the coherent states for N degrees of freedom by repeated application to the multiple vacuum state

$$|\alpha_1, \alpha_2, \ldots, \alpha_N\rangle = \prod_{i=1}^{N} D(\alpha_i)|0, \ldots, 0\rangle \tag{533}$$

for $\alpha_i \in \mathbb{Z}$, $i = 1, \ldots, N$.

3. Saturation of the Uncertainty Relation:
For an arbitrary state $|\psi\rangle$ which we will shortly denote by $\rangle$ the ***standard deviation*** $\Delta\hat{o}$ of an operator $\hat{o}$ is defined by

$$(\Delta\hat{o}) := \sqrt{\langle\hat{o}^2\rangle - \langle\hat{o}\rangle^2}. \tag{534}$$

The standard ***uncertainty relation*** is given by

$$(\Delta\hat{q})\,(\Delta\hat{p}) \geq \frac{\hbar}{2}. \tag{535}$$

Now the coherent states $|\alpha\rangle$, or even $|\alpha, t\rangle$ for a general time parameter t displayed below, are exactly those states which minimize the uncertainty relation, that is

$$(\Delta\hat{q})\,(\Delta\hat{p}) = \frac{\hbar}{2}. \tag{536}$$

For the time-independent harmonic oscillator all three ways lead to the same coherent states but for different physical systems this might not be the case, see for example [32].

14.3 Stability of the H.O. Coherent States

Let us recall how the time-dependent coherent states $|\alpha, t\rangle$ can be obtained from the time-independent coherent states $|\alpha\rangle$ by application of the unitary time-evolution operator $\hat{U}(t)$ to $|\alpha\rangle$ which yields

$$\begin{aligned} |\alpha, t\rangle &:= \hat{U}(t)|\alpha\rangle = e^{-\frac{i}{\hbar}\hat{H}_{\mathrm{ho}}t}|\alpha\rangle \\ &= e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\omega_0(n+\frac{1}{2})t}|n\rangle \\ &= e^{-\frac{i}{2}\omega_0 t}|\alpha(t)\rangle. \end{aligned} \tag{537}$$

with $\alpha(t) := \alpha\, e^{-i\omega_0 t}$.

We calculate the expectation values of the position and momentum operators in the coherent and time-evolved coherent states leading to

$$\begin{aligned} \langle\alpha|\hat{q}|\alpha\rangle &= \sqrt{\frac{2\hbar}{m\omega_0}}\Re(\alpha) = \sqrt{\frac{2\hbar}{m\omega_0}}|\alpha|\cos(\delta), \\ \langle\alpha|\hat{p}|\alpha\rangle &= \sqrt{2m\hbar\omega_0}\Im(\alpha) = -\sqrt{2m\hbar\omega_0}|\alpha|\sin(\delta) \end{aligned} \tag{538}$$

and

$$\begin{aligned} \langle\alpha, t|\hat{q}|\alpha, t\rangle &= \sqrt{\frac{2\hbar}{m\omega_0}}\Re(\alpha(t)) = \sqrt{\frac{2\hbar}{m\omega_0}}|\alpha|\cos(\omega_0 t + \delta), \\ \langle\alpha, t|\hat{p}|\alpha, t\rangle &= \sqrt{2m\hbar\omega_0}\Im(\alpha(t)) = -\sqrt{2m\hbar\omega_0}|\alpha|\sin(\omega_0 t + \delta) \end{aligned} \tag{539}$$

with $\alpha = |\alpha|e^{-i\delta}$, $\delta \in \mathbb{R}$. Eq. (539) means that the expectation values of the position $\hat{q}$ and momentum operator $\hat{p}$ in the states $|\alpha\rangle$ or $|\alpha, t\rangle$, which correspond to the centre of the wave package, follow the classical trajectories $q(t)$ and $p(t)$ for all times t. This is ensured because the time evolution of the coherent states in eq. (537) is carried over to the label α which is related to the classical phase space variables q and p via $\alpha = \sqrt{\frac{m\omega_0}{2\hbar}}q + i\frac{1}{\sqrt{2\hbar m\omega_0}}p$.

So we see that the harmonic oscillator coherent states work well for the time-independent harmonic oscillator they were constructed for. This brings us to the question what will happen, if we consider a modification of the harmonic oscillator. Since we are interested in square roots, as a toy model we consider the square root of the time-independent harmonic oscillator

$$\hat{H}_{\mathrm{sqrt}} = \sqrt{\frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0^2\hat{q}^2} = \sqrt{\hbar\omega_0\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\mathbb{1}\right)}. \tag{540}$$

The calculation of the expectation value of $\hat{H}_{\mathrm{sqrt}}$ in the standard harmonic oscillator coherent states $|\alpha\rangle$ leads to

$$\langle\alpha|\hat{H}_{\mathrm{sqrt}}|\alpha\rangle = \langle\alpha, t|\hat{H}_{\mathrm{sqrt}}|\alpha, t\rangle = e^{-|\alpha|^2}\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!}\sqrt{\hbar\omega_0\left(n + \frac{1}{2}\right)} \tag{541}$$

which is not what we would expect classically. To get an idea of what kind of problems for the square root Hamiltonian arise, we can also apply the evolution operator based on $\hat{H}_{\mathrm{sqrt}}$ to $|\alpha\rangle$ which results in

$$e^{-\frac{i}{\hbar}\hat{H}_{\mathrm{sqrt}}t}|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-\frac{i}{\hbar}\sqrt{\hbar\omega_0(n+\frac{1}{2})}t}|n\rangle. \tag{542}$$

This naive ansatz does not bring us too far. However, what we see from these calculations is that the linearity of a Hamilton operator in the number operator $\hat{n}$ is really a special case which simplifies many calculations, since now we are not able to split the n-term in eq. (541) or the exponential in eq. (542) to simplify the expressions.

15 Inverse Thiemann Identity for Square Root Hamiltonians

We can also try to avoid the square root right from the beginning, that is before we attempt to quantize the system by finding a kind of effective Hamiltonian replacement for the original square root Hamiltonian. We will also come back to this idea at the end of this part in section 22 in a different context. For now we start with the classical square root Hamiltonian and apply what we will in the following call the ***"inverse Thiemann identity"***. After the application of the inverse Thiemann identity we will quantize the simplified expression. Let the Hamiltonians for the time-independent harmonic oscillator H_{ho} and for the square root H_{sqrt} of it as before be given by

$$H_{\mathrm{ho}} = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2q^2, \quad H_{\mathrm{sqrt}} := \sqrt{H_{\mathrm{ho}}}. \tag{543}$$

Then the classical Hamiltonian equations of motion follow from the Poisson brackets of the position variable q and momentum variable p with the Hamiltonian. We will apply the inverse

Thiemann identity to modify them in such a way that they become

$$\begin{aligned} \dot{q} &= \{q, H_{\text{sqrt}}\} = \frac{1}{2\sqrt{H_{\text{ho}}}}\{q, H_{\text{ho}}\} = \frac{1}{2H_{\text{sqrt}}}\frac{p}{m}, \\ \dot{p} &= \{p, H_{\text{sqrt}}\} = \frac{1}{2\sqrt{H_{\text{ho}}}}\{p, H_{\text{ho}}\} = -\frac{1}{2H_{\text{sqrt}}}qm\omega_0^2. \end{aligned} \tag{544}$$

The inverse Thiemann identity means that instead of considering H_{sqrt} in the Poisson bracket during the quantization process, we use the understanding of the Poisson bracket as differentiation, which follows from its definition, and consider the outcome of the Poisson brackets of q and p with H_{ho} as quantities that can be quantized. The Thiemann identity is actually applied in LQG to be able to quantize the Hamiltonian constraint, compare part II. Here we used the addition "inverse", since there one uses it to substitute an non quantizable quantity by a Poisson bracket, whereas here we use it to substitute a quantity in a Poisson bracket. With this we obtain

$$\begin{aligned} \ddot{q} &= \frac{1}{2H_{\text{sqrt}}}\frac{\dot{p}}{m} = -\frac{1}{4H_{\text{sqrt}}^2}\frac{qm\omega_0^2}{m} = -\left(\frac{\omega_0}{2H_{\text{sqrt}}}\right)^2 q \\ &\Leftrightarrow \ddot{q} + \Omega^2 q = 0 \end{aligned} \tag{545}$$

with $\Omega := \Omega(E_{\text{sqrt}})^2 := \left(\frac{\omega_0}{2H_{\text{sqrt}}}\right)^2 = \frac{\omega_0^2}{4E_{\text{sqrt}}^2}$, where we assume that classically H_{sqrt} is the energy E_{sqrt} of our toy model. This is the well known equation of motion for a time-independent harmonic oscillator with modified frequency Ω.

15.1 Effective Hamiltonian

If we want to go over to the quantum theory, the question will arise how to fix $\Omega(E_{\text{sqrt}})$. We may do it in a semiclassical way in the sense that we consider Ω as a function of the expectation value of $\hat{H}_{\text{sqrt}}$ and demand it to be equal to the energy E_{sqrt} of the classical system, that is $\Omega(\langle\hat{H}_{\text{sqrt}}\rangle) = \Omega(E_{\text{sqrt}})$. For $\hat{H}_{\text{sqrt}}$ we know that this will work out, in case that we take the expectation value of $\hat{H}_{\text{sqrt}}$ in the number operator eigenstates $|n\rangle$. In this semiclassical sense, the frequency Ω becomes

$$\Omega(E_{\text{sqrt}}) = \frac{\omega_0}{\langle\hat{H}_{\text{sqrt}}\rangle} = \frac{\omega_0}{\sqrt{\hbar\omega_0\left(n+\frac{1}{2}\right)}} = \frac{\omega_0}{\sqrt{\frac{1}{2m}p_0^2 + \frac{m}{2}q_0^2\omega_0^2}} = \Omega(q_0, p_0) \tag{546}$$

with $n \in \mathbb{N}_0$. The zero index here is meant to remind us that for a certain energy value of E_{sqrt} Ω depends on the phase space point (q_0, p_0).

Next we will define an effective Hamiltonian operator $\hat{H}_E$ in analogy to the standard harmonic oscillator, where we consider $H_{\text{sqrt}} = E_{\text{sqrt}}$ in Ω as explained in eq. (546) classically, however regard q and p as operators. In correspondence with the definition of the standard time-independent harmonic oscillator, we can define the new annihilation and creation operators

$$\hat{A} = \sqrt{\frac{m\Omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\Omega}\hat{p}\right), \quad \hat{A}^\dagger = \sqrt{\frac{m\Omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\Omega}\hat{p}\right) \tag{547}$$

They can be formulated in terms of the standard harmonic oscillator annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$ as

$$\hat{A} = \frac{1}{2}\sqrt{\frac{\Omega}{\omega_0}}\left[\left(1+\frac{\omega_0}{\Omega}\right)\hat{a} + \left(1-\frac{\omega_0}{\Omega}\right)\hat{a}^\dagger\right], \quad \hat{A}^\dagger = \frac{1}{2}\sqrt{\frac{\Omega}{\omega_0}}\left[\left(1+\frac{\omega_0}{\Omega}\right)\hat{a}^\dagger + \left(1-\frac{\omega_0}{\Omega}\right)\hat{a}\right]. \quad (548)$$

One can easily see that they satisfy the commutation relation

$$\left[\hat{A}, \hat{A}^\dagger\right] = \hat{\mathbb{1}}. \quad (549)$$

With this the effective Hamiltonian operator can be expressed as

$$\hat{H}_E = \hbar\Omega\left(\hat{A}^\dagger\hat{A} + \frac{1}{2}\hat{\mathbb{1}}\right). \quad (550)$$

From the equation of motion in eq. (545), we expect that we should be able to use the standard harmonic oscillator coherent states to calculate the expectation value of $\hat{H}_E$ and obtain as a result the classical Hamiltonian of a harmonic oscillator with modified frequency. However, due to our classical consideration of the modified frequency, that actually involves H_{sqrt}, we see that $\hat{A}$ and $\hat{A}^\dagger$ include sums of $\hat{a}$ and $\hat{a}^\dagger$ which tells us that it makes no sense to use the standard harmonic oscillator coherent states.

In fact, if we calculate the expectation value of $\hat{H}_E$ in the standard harmonic oscillator coherent states $|\alpha\rangle$, we will find that

$$\langle\alpha|\hat{H}_E|\alpha\rangle = \frac{\hbar}{4}\frac{\Omega^2}{\omega_0}\left[2\left(1+\frac{\omega_0^2}{\Omega^4}\right)|\alpha|^2 + \left(1-\frac{\omega_0^2}{\Omega^4}\right)\left(\alpha^2+(\alpha^*)^2\right) + \left(1-\frac{\omega_0^2}{\Omega^4}\right)\right]. \quad (551)$$

Now let us define

$$u = u^* := \frac{1}{2}\sqrt{\frac{\Omega}{\omega_0}}\left(1+\frac{\omega_0}{\Omega}\right), \quad v = v^* := \frac{1}{2}\sqrt{\frac{\Omega}{\omega_0}}\left(1-\frac{\omega_0}{\Omega}\right), \quad (552)$$

then we can see that $\hat{A}$ and $\hat{A}^\dagger$ in eq. (548) arise from $\hat{a}$ and $\hat{a}^\dagger$ by a ***Bogoliubov transformation***, since we can write

$$\hat{A} = u\hat{a} + v\hat{a}^\dagger, \quad \hat{A}^\dagger = u^*\hat{a}^\dagger + v^*\hat{a} \quad (553)$$

and check that $|u|^2 - |v|^2 = 1$. In our case u and v are real.

It is possible to express u and v as

$$u := \cosh(r), \quad v := \sinh(r), \quad (554)$$

where $r \in \mathbb{R}$ is the so-called ***squeezing factor***. Below we will show that a kind of so-called squeezed states are eigenstates of $\hat{A}$, compare for example [143] and [144].

A squeezed state is a state which satisfies the minimal uncertainty relation but the standard deviations Δq and Δp calculated in a squeezed state do not have identical values and oscillate, for details see [145, 146]. It is the first generalization of the harmonic oscillator coherent state $|\alpha\rangle$ gained from the application of the displacement operator to the vacuum state $|0\rangle$ of the harmonic oscillator. The ***squeezed state*** is defined as

$$|\alpha, z\rangle := \hat{D}(\alpha)\hat{S}(z)|0\rangle = \hat{S}(z)\hat{D}(\gamma)|0\rangle, \quad \gamma = \alpha\cosh(r) - \alpha^* e^{i\theta}\sinh(r) \quad (555)$$

with displacement operator $\hat{D}(\alpha)$ compare eq. (531) and ***squeezing operator*** $\hat{S}(z)$ given by

$$\hat{S}(z) := \exp\left[\frac{1}{2}\left(z(\hat{a}^\dagger)^2 - z^*\hat{a}^2\right)\right] \quad (556)$$

for $z = re^{i\theta}$, $-\infty < r < \infty$, $-\pi < \theta \leq \pi$ and $\alpha \in \mathbb{C}$. One can easily check that $\hat{S}^\dagger(z) = \hat{S}^{-1}(z) = \hat{S}(-z)$. Depending on the kind of physical application also the state gained from the reversed application of $\hat{D}(\alpha)$ and $\hat{S}(z)$ can be found in the literature, however notice that the order of the operators applied to $|0\rangle$ matters, i.e. $\hat{S}(z)\hat{D}(\alpha)|0\rangle \neq \hat{D}(\alpha)\hat{S}(z)|0\rangle$ which is also discussed in [145]. One can use the squeezing operator to perfom unitary transformations of $\hat{a}$ and $\hat{a}^\dagger$ to $\hat{A}$ or $\hat{A}^\dagger$ by

$$\begin{aligned} \hat{A} &= \hat{S}^\dagger(z)\hat{a}\hat{S}(z) = \cosh(r)\hat{a} + \sinh(r)\hat{a}^\dagger, \\ \hat{A}^\dagger &= \hat{S}^\dagger(z)\hat{a}^\dagger\hat{S}(z) = \cosh(r)\hat{a}^\dagger + \sinh(r)\hat{a}, \end{aligned} \tag{557}$$

where we set $\theta = 0$. By using $-z$ instead of z in the definition for the squeezed state, we can see that $|\alpha, -z\rangle$ is an eigenstate for $\hat{A}$, namely

$$\begin{aligned} \hat{A}|\alpha, -z\rangle &= \hat{S}^\dagger(z)\hat{a}\hat{S}(z)\hat{D}(\alpha)\hat{S}(-z)|0\rangle \\ &= \hat{S}^\dagger(z)\hat{a}\hat{S}(z)\hat{S}^\dagger(z)\hat{D}(\gamma)|0\rangle \\ &= \hat{S}^\dagger(z)\hat{a}\hat{D}(\gamma)|0\rangle \\ &= \hat{S}^\dagger(z)\gamma\hat{D}(\gamma)|0\rangle \\ &= \gamma\hat{S}(-z)\hat{D}(\gamma)|0\rangle \\ &= \gamma\hat{D}(\alpha)\hat{S}(-z)|0\rangle = \gamma|\alpha, -z\rangle, \end{aligned} \tag{558}$$

where we used that $\hat{S}(-z) = \hat{S}^\dagger(z) = \hat{S}^{-1}(z)$ and $\gamma = \alpha\cosh(r) - \alpha^*\sinh(r) = \alpha u - \alpha^* v$ with $\theta = 0$. The expectation value of $\hat{H}_E$ in the squeezed states $|\alpha, -z\rangle$ becomes

$$\begin{aligned} \langle\alpha, -z|\hat{H}_E|\alpha, -z\rangle &= \hbar\Omega\left(|\gamma|^2 + \frac{1}{2}\right) = \hbar\Omega\left(|\alpha|^2\left(u^2 + v^2\right) - uv\left[(\alpha^*)^2 + \alpha^2\right] + \frac{1}{2}\right) \\ &= \hbar\Omega\left(|\alpha|^2\left(\cosh(r)^2 + \sinh(r)^2\right) - \cosh(r)\sinh(r)\left[(\alpha^*)^2 + \alpha^2\right] + \frac{1}{2}\right) \\ &= \frac{\hbar}{4}\frac{\Omega^2}{\omega_0}\left[2\left(1 + \frac{\omega_0^2}{\Omega^2}\right)|\alpha|^2 - \left(1 - \frac{\omega_0^2}{\Omega^2}\right)\left(\alpha^2 + (\alpha^*)^2\right) + 2\frac{\omega_0}{\Omega}\right]. \end{aligned} \tag{559}$$

We can calculate r from

$$\begin{aligned} r = \operatorname{arsinh}(v) &= \ln\left(v + \sqrt{v^2 + 1}\right) = \ln\left(\frac{1}{2}\sqrt{\frac{\Omega}{\omega_0}}\left(1 - \frac{\omega_0}{\Omega}\right) + \sqrt{\frac{1}{4}\frac{\Omega}{\omega_0}\left(1 - \frac{\omega_0}{\Omega}\right)^2 + 1}\right) \\ &= \ln\left(\sqrt{\frac{\Omega}{\omega_0}}\right) = -\frac{1}{2}\ln\left(\frac{\omega_0}{\Omega}\right) \end{aligned} \tag{560}$$

and $\left(v + \sqrt{v^2 + 1}\right) \in (0, \infty)$ which is given since $\frac{\omega_0}{\Omega} = 2\sqrt{\hbar\omega_0(n + \frac{1}{2})} > 0$ for $n \in \mathbb{N}_0$. Reinserting this r into $\sinh(r)$ and $\cosh(r)$ reproduces v and u.

Despite that $|\alpha, -z\rangle$ is an eigenstate of $\hat{A}$, eq. (559) shows that it is not well-adapted to the effective Hamiltonian operator in a semiclassical sense because the expectation value of the effective Hamiltonian operator in squeezed states does not reproduce the classical value of the harmonic oscillator with modified frequency.

We conclude that though the idea to rewrite the square root on the classical level seems appealing, it does not bring us too far, since our classical treatment of the frequency Ω while we lift the position q and momentum p to the operator level did not help us to find appropriate semiclassical states. Actually, what we did in this section resulted in a modification of the underlying operator, but we did not adapt the construction method to the square root Hamiltonian itself. In the upcoming sections instead of replacing the square root operator, we really want to modify the states.

As mentioned in the introduction to this section, the idea of an effective Hamiltonian will encounter us again in section 22, however there we will use a different procedure called Euler rescaling in combination with an enlargement of the underlying phase space and also choose an adapted construction for the semiclassical states.

16 Phase Operators and Phase States

Our aim is to find ways to handle the square root of the harmonic oscillator Hamiltonian, shortly denoted as square root Hamiltonian. In section 15 we tried to circumvent the square root by defining an effective Hamiltonian, however this did not bring us too far and we did not construct better adapted states. Now we want to make a transition to tackle the problem from a different side, namely from the algebraic one. In [40] Daoud and Kibler introduce a generalized one-parameter algebra $\mathfrak{A}_\kappa$, where κ is a real parameter, as a generalization of the harmonic oscillator (Weyl-Heisenberg) algebra. The algebra $\mathfrak{A}_\kappa$ has finite- or infinite-dimensional representations depending on the sign of κ (finite for $\kappa < 0$ and infinite for $\kappa \geq 0$). A Hamiltonian operator associated with $\mathfrak{A}_\kappa$ was constructed and its spectrum was examined. To work around difficulties related with definedness in the infinite-dimensional case and degeneracy in the finite-dimensional case, in their article [40] they introduce a truncation procedure such that they finally gain a truncated generalized oscillator algebra $\mathfrak{A}_{\kappa,s}$ with truncation order s. For $\mathfrak{A}_\kappa$ and $\mathfrak{A}_{\kappa,s}$ the related phase operators and temporally stable phase states were constructed. The origin of the considered generalized harmonic oscillator algebra $\mathfrak{A}_\kappa$ lies in the construction of so-called isospectral shape invariant potentials in the framework of fractional SUSY, see for example [34].

Now we want to explain how to use and modify their methods to apply them to our problem of the square root Hamiltonian.

16.1 Generalized Oscillator Algebra

Let us summarize the main results of [40]. The algebra $\mathfrak{A}_\kappa$ is spanned by the three linear boson operators $\hat{a}^-$, $\hat{a}^+$ and $\hat{n}$ which satisfy the commutation relations

$$\left[\hat{a}^-, \hat{a}^+\right] = \hat{\mathbb{1}} + 2\kappa\hat{n}, \quad \left[\hat{n}, \hat{a}^\pm\right] = \pm\hat{a}^\pm \tag{561}$$

with $(\hat{a}^-)^\dagger = \hat{a}^+$, $\hat{n}^\dagger = \hat{n}$ and a real parameter κ. The operators $\hat{a}^-$ and $\hat{a}^+$ generalize the usual annihilation and creation operators of the harmonic oscillator. For $\kappa = 0$ we have the ordinary harmonic oscillator algebra, the so-called ***Weyl-Heisenberg algebra*** wh. So $\mathfrak{A}_\kappa$ is a generalization of the Weyl-Heisenberg algebra wh. Let $\mathcal{H}_\kappa$ be the finite or infinite dimensional Hilbert space with respect to the inner product $\langle n|n'\rangle = \delta_{nn'}$ on which $\hat{a}^-$, $\hat{a}^+$ and $\hat{n}$ are defined and define an orthonormal basis by $\{|n\rangle : n = 0, 1, \dots, d(\kappa)\}$, where $d(\kappa)$ is the dimension of the Hilbert space. A representation of the algebra $\mathfrak{A}_\kappa$ is provided by, see [40],

$$\begin{aligned}
&\hat{n}|n\rangle = n|n\rangle, \\
&\hat{a}^+|n\rangle = \sqrt{F(n+1)}e^{-i[F(n+1)-F(n)]\varphi}|n+1\rangle, \\
&\hat{a}^-|n\rangle = \sqrt{F(n)}e^{i[F(n)-F(n-1)]\varphi}|n-1\rangle, \\
&\hat{a}^-|0\rangle = 0
\end{aligned} \tag{562}$$

with a real parameter φ and a positively-valued function $F : \mathbb{N} \to \mathbb{R}_+^0$ which satisfies

$$F(n+1) - F(n) = 1 + 2\kappa n, \quad F(0) = 0. \tag{563}$$

An iteration of this expression leads to

$$F(n) = n\left[1 + \kappa\,(n-1)\right] \tag{564}$$

and since $F(n) \in \mathbb{R}_+^0$ we need to fulfill the condition $1 + \kappa\,(n-1) > 0$ for $n > 0$.

Now we can define a Hamiltonian operator $F(\hat{n})$ associated with the algebra $\mathfrak{A}_\kappa$ which is up to a constant a generalization of the usual one-dimensional harmonic oscillator Hamiltonian operator $\hat{H}_{\text{ho}} = \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{\mathbb{1}}\right)$, where we set $\hbar\omega_0 = 1$. From

$$\hat{a}^+\hat{a}^-|n\rangle = F(n)|n\rangle \tag{565}$$

we obtain

$$F(\hat{n}) = \hat{a}^+\hat{a}^- \tag{566}$$

and

$$F(\hat{n})|n\rangle = n\left[1 + \kappa\,(n-1)\right]|n\rangle = F(n)|n\rangle =: E_n|n\rangle \tag{567}$$

gives the energies E_n of a quantum dynamical system described by $F(\hat{n})$.

To obtain the spectrum of $F(\hat{n})$ we have to consider the two cases :

(i) Case $\kappa \geq 0$, the spectrum of $F(\hat{n})$ is non-degenerate.

(ii) Case $\kappa < 0$, the spectrum of $F(\hat{n})$ is degenerate.

16.2 Phase States for $\mathfrak{A}_\kappa$

Infinite-dimensional case:
We consider the case where $\kappa \geq 0$ and decompose $\hat{a}^-$ and $\hat{a}^+$ as

$$\hat{a}^- = \hat{E}_\infty\sqrt{F(\hat{n})}, \quad \hat{a}^+ = \sqrt{F(\hat{n})}\left(\hat{E}_\infty\right)^\dagger \tag{568}$$

with

$$\hat{E}_\infty := \sum_{n=0}^{\infty} e^{i[F(n+1)-F(n)]\varphi}|n\rangle\langle n+1|, \tag{569}$$

where $\hat{E}_\infty$ is the so-called ***phase operator***. Notice that the phase operator $\hat{E}_\infty$ is not a unitary operator, since

$$\begin{aligned}\hat{E}_\infty\left(\hat{E}_\infty\right)^\dagger &= \sum_{n=0}^{\infty}|n\rangle\langle n| = \hat{\mathbb{1}}, \\ \left(\hat{E}_\infty\right)^\dagger\hat{E}_\infty &= \sum_{n=0}^{\infty}|n\rangle\langle n| = \hat{\mathbb{1}} - |0\rangle\langle 0|.\end{aligned} \tag{570}$$

Next we want to construct the phase states $|z\rangle$ which are eigenstates of the phase operator according to the eigenvalue equation

$$\hat{E}_\infty|z\rangle = z|z\rangle, \quad z \in \mathbb{C}. \tag{571}$$

We expand $|z\rangle \in \mathcal{H}_\kappa$ in the basis $|n\rangle$ which is

$$|z\rangle = \sum_{n=0}^{\infty} C_n z^n |n\rangle \tag{572}$$

with coefficients $C_n \in \mathbb{C}$, $n \in \mathbb{N}_0$. From

$$\begin{aligned}
\hat{E}_\infty|z\rangle &= \sum_{k=0}^{\infty}\sum_{m=0}^{\infty} e^{i[F(k+1)-F(k)]\varphi} C_m z^m |k\rangle \underbrace{\langle k+1|m\rangle}_{\delta_{k+1,m}} \\
&= \sum_{k=0}^{\infty} e^{i[F(k+1)-F(k)]\varphi} C_{k+1} z^{k+1} |k\rangle \\
&= z\sum_{k=0}^{\infty} e^{i[F(k+1)-F(k)]\varphi} C_{k+1} z^{k} |k\rangle \\
&= z|z\rangle = z\sum_{k=0}^{\infty} C_k z^k |k\rangle
\end{aligned} \tag{573}$$

we see that the coefficients C_n can be derived from the recursive relation

$$C_{n+1} = e^{-i[F(n+1)-F(n)]\varphi} C_n, \quad n \in \mathbb{N}_0,$$

which leads to

$$C_n = e^{-iF(n)\varphi} C_0, \tag{574}$$

where $C_0 = \sqrt{1-|z|^2}$ for $\{z \in \mathbb{C}, |z| < 1\}$ follows from a normalization condition on $|z\rangle$ that requires the appearing series to converge.

Then the state for $|z\rangle$, up to a phase factor, is given by the expression

$$|z\rangle = \sqrt{1-|z|^2}\sum_{n=0}^{\infty} e^{-iF(n)\varphi} z^n |n\rangle \tag{575}$$

on the domain $\{z \in \mathbb{C}, |z| < 1\}$. Following a method developed in [147] for the Lie algebra $su(1,1)$ one can define the so-called ***phase states*** $|\theta,\varphi\rangle$ by

$$|\theta,\varphi\rangle := \lim_{z\to e^{i\theta}} \frac{1}{\sqrt{1-|z|^2}}|z\rangle, \quad -\pi \le \theta < \pi. \tag{576}$$

Plugging in the expression for $|z\rangle$, we end up with

$$|\theta,\varphi\rangle = \sum_{n=0}^{\infty} e^{in\theta} e^{-iF(n)\varphi}|n\rangle, \quad -\pi \le \theta < \pi, \tag{577}$$

defined on the unit circle S^1. For fixed φ the phase states satisfy a resolution of identity, see for instance [41], given by

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta|\theta,\varphi\rangle\langle\theta,\varphi| = \hat{\mathbb{1}}, \tag{578}$$

however they are neither normalizable nor orthogonal.

If we apply $\hat{E}_\infty$ to the state $|\theta,\varphi\rangle$ which yields

$$\hat{E}_\infty|\theta,\varphi\rangle = e^{i\theta}|\theta,\varphi\rangle, \quad -\pi \leq \theta < \pi, \tag{579}$$

we will see that the non-unitary phase operator $\hat{E}_\infty$ applied to the state $|\theta,\varphi\rangle$ has the eigenvalue $e^{i\theta}$ which makes it obvious why it is called phase operator.

Let us collect some ***properties of the phase states*** $|\theta,\varphi\rangle$ ***:***

1. The phase states are temporally stable in the sense that

$$e^{-iF(\hat{n})t}|\theta,\varphi\rangle = \sum_{n=0}^{\infty} e^{in\theta}e^{-iF(n)(\varphi+t)}|n\rangle = |\theta,\varphi+t\rangle \tag{580}$$

   for any parameter $t \in \mathbb{R}$ and $\hbar = 1$.

2. In general they are not normalized and not orthogonal but for fixed φ we have

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta\,|\theta,\varphi\rangle\langle\theta,\varphi| = \hat{\mathbb{1}}. \tag{581}$$

3. They are no eigenstates of the annihilation operator, since

$$\hat{a}^-|\theta,\varphi\rangle = e^{i\theta}\sum_{n=0}^{\infty} \sqrt{F(n+1)}e^{in\theta}e^{-iF(n)\varphi}|n\rangle. \tag{582}$$

Finite-dimensional case:
We will leave the description of the finite-dimensional case for $\kappa < 0$ out here because we will not use it. The definition of the truncated algebra $\mathfrak{A}_{\kappa,s}$ and further details for the case $\kappa < 0$ can be found in [40].

As a remark, notice that for $\varphi = 0$ one obtains the same states as derived for $\mathrm{SU}(1,1)$ in [41], where complete applications of these techniques to $\mathrm{SU}(2)$ ($\kappa < 0$) and $\mathrm{SU}(1,1)$ ($\kappa \geq 0$) can be found.

16.3 Application to the Square Root Hamiltonian

The techniques discussed in [40] were not developed to handle Hamiltonians including a square root. Despite that we can apply them in a slightly modified form to our toy model of the square root of the harmonic oscillator. We are in the case $\kappa = 0$ and make the ansatz

$$\sqrt{\hat{a}^+\hat{a}^-}|n\rangle = F(n)|n\rangle, \tag{583}$$

where we neglect the constant $\frac{1}{2}$ term. Following [40] we have

$$F(\hat{n}) = \sqrt{\hat{n}} = \sqrt{\hat{a}^+\hat{a}^-} \tag{584}$$

with the annihilation and creation operators $\hat{a}^-$ and $\hat{a}^+$ defined by

$$\begin{aligned} \hat{a}^- &:= \hat{E}_\infty \sqrt{F(\hat{n})} = \hat{E}_\infty \hat{n}^{\frac{1}{4}}, \\ \hat{a}^+ &:= \sqrt{F(\hat{n})} \left(\hat{E}_\infty\right)^\dagger = \hat{n}^{\frac{1}{4}} \left(\hat{E}_\infty\right)^\dagger \end{aligned} \tag{585}$$

and the phase operator $\hat{E}_\infty$ in this case reads

$$\hat{E}_\infty = \sum_{n=0}^{\infty} e^{i[F(n+1)-F(n)]\varphi} |n\rangle\langle n+1| = \sum_{n=0}^{\infty} e^{i\left[\sqrt{n+1}-\sqrt{n}\right]\varphi} |n\rangle\langle n+1| \tag{586}$$

for $\varphi \in \mathbb{R}$. However, now the classical condition becomes $F(n+1) - F(n) = \sqrt{n+1} - \sqrt{n} \neq 1$, therefore we are strictly not in the case of [40]. This is reflected in the algebra which now changes to

$$\left[\hat{a}^-, \hat{a}^+\right] = \sum_{n=0}^{\infty} \left(\sqrt{n+1} - \sqrt{n}\right) |n\rangle\langle n|, \quad \left[\hat{n}, \hat{a}^\pm\right] = \pm\hat{a}^\pm. \tag{587}$$

Yet another inconsistency will show up, if we make the following calculation

$$\begin{aligned} \sqrt{\hat{n}}|n\rangle &= \sqrt{\hat{a}^+\hat{a}^-}|n\rangle = \sqrt{\hat{n}^{\frac{1}{4}} \left(\hat{E}_\infty\right)^\dagger \hat{E}_\infty \hat{n}^{\frac{1}{4}}}|n\rangle \\ &= \sqrt{\hat{n}^{\frac{1}{4}} \left(\hat{\mathbb{1}} - |0\rangle\langle 0|\right) \hat{n}^{\frac{1}{4}}}|n\rangle = \sqrt{\hat{n}^{\frac{1}{4}} n^{\frac{1}{4}}}|n\rangle \\ &= \sqrt{n^{\frac{1}{2}}}|n\rangle = \sqrt{\sqrt{n}|n\rangle} \neq \sqrt{n}|n\rangle. \end{aligned} \tag{588}$$

This can easily be fixed by redefining $\hat{a}^-$ and $\hat{a}^+$ to

$$\hat{a}^- := \hat{E}_\infty F(\hat{n}), \quad \hat{a}^+ := F(\hat{n}) \left(\hat{E}_\infty\right)^\dagger. \tag{589}$$

Additionally, the re-definition solves our problem with the algebra which modifies to

$$\left[\hat{a}^-, \hat{a}^+\right] = \hat{\mathbb{1}}, \quad \left[\hat{n}, \hat{a}^\pm\right] = \pm\hat{a}^\pm \tag{590}$$

and hence is isomorphic to the Weyl-Heisenberg algebra. The definition of the phase operator $\hat{E}_\infty$ stays unchanged. A short calculation shows that

$$\begin{aligned} \hat{E}_\infty \left(\hat{E}_\infty\right)^\dagger &= \sum_{k=0}^{\infty} e^{i\left[\sqrt{k+1}-\sqrt{k}\right]\varphi} |k\rangle\langle k+1| \sum_{m=0}^{\infty} e^{-i\left[\sqrt{m+1}-\sqrt{m}\right]\varphi} |m+1\rangle\langle m| \\ &= \sum_{k=0}^{\infty}\sum_{m=0}^{\infty} e^{i\left[\sqrt{k+1}-\sqrt{k}-\sqrt{m+1}+\sqrt{m}\right]\varphi} |k\rangle \underbrace{\langle k+1|m+1\rangle}_{\delta_{m+1,k+1}=\delta_{m,k}} \langle m| \\ &= \sum_{k=0}^{\infty} |k\rangle\langle k| = \hat{\mathbb{1}} \end{aligned} \tag{591}$$

and

$$\left(\hat{E}_\infty\right)^\dagger \hat{E}_\infty = \sum_{m=0}^{\infty} e^{-i\left[\sqrt{m+1}-\sqrt{m}\right]\varphi}|m+1\rangle\langle m| \sum_{k=0}^{\infty} e^{i\left[\sqrt{k+1}-\sqrt{k}\right]\varphi}|k\rangle\langle k+1| \tag{592}$$

$$= \sum_{m=0}^{\infty}\sum_{k=0}^{\infty} e^{-i\left[\sqrt{m+1}-\sqrt{m}-\sqrt{k+1}+\sqrt{k}\right]\varphi}|m+1\rangle \underbrace{\langle m|k\rangle}_{\delta_{m,k}} \langle k+1|$$

$$= \sum_{k=0}^{\infty} |k+1\rangle\langle k+1| = \sum_{k=0}^{\infty} |k\rangle\langle k| - |0\rangle\langle 0| = \hat{\mathbb{1}} - |0\rangle\langle 0|$$

which tells us that also here the phase operator $\hat{E}_\infty$ is, as expected, not unitary. The phase states for our square root Hamiltonian read

$$|\theta,\varphi\rangle = \sum_{n=0}^{\infty} e^{in\theta} e^{-iF(n)\varphi}|n\rangle = \sum_{n=0}^{\infty} e^{in\theta}e^{-i\sqrt{n}\varphi}|n\rangle. \tag{593}$$

Now we want to check whether the gained phase states are temporally stable in the sense explained in eq. (580). Therefore, we calculate

$$e^{-i\sqrt{\hat{n}}t}|\theta,\varphi\rangle = e^{-i\sqrt{\hat{n}}t}\sum_{n=0}^{\infty} e^{in\theta}e^{-i\sqrt{n}\varphi}|n\rangle = \sum_{n=0}^{\infty} e^{in\theta}e^{-i\sqrt{n}\varphi}e^{-i\sqrt{n}t}|n\rangle \tag{594}$$

$$= \sum_{n=0}^{\infty} e^{in\theta}e^{-i\sqrt{n}(\varphi+t)}|n\rangle = |\theta,\varphi+t\rangle.$$

In the re-definition of $\hat{a}^-$ and $\hat{a}^+$ we only consider $F(\hat{n}) = \sqrt{\hat{n}}$ instead of $\sqrt{F(\hat{n})} = \sqrt{\sqrt{\hat{n}}}$. The re-definition of $\hat{a}^-$ and $\hat{a}^+$ does not influence the calculations using the definitions of the phase operator $\hat{E}_\infty$ and the phase states $|\theta,\varphi\rangle$, since the phase operator $\hat{E}_\infty$ and the phase states $|\theta,\varphi\rangle$ are not influenced by this. It seems that we actually get some stable states in the sense explained in [40]. Though, the phase states are only defined on the unit circle S^1.

To check whether the expectation values in the phase states reproduce the classical values in general, we calculate the expectation values

$$\langle\theta,\varphi|\hat{a}^-|\theta,\varphi\rangle = e^{i\theta}\sum_{n=1}^{\infty}\sqrt{F(n)}, \quad \langle\theta,\varphi|\hat{a}^+|\theta,\varphi\rangle = e^{-i\theta}\sum_{n=1}^{\infty}\sqrt{F(n)}, \tag{595}$$

$$\langle\theta,\varphi|F(\hat{n})|\theta,\varphi\rangle = \sum_{n=1}^{\infty} F(n), \quad \langle\theta,\varphi|\hat{E}_\infty|\theta,\varphi\rangle = e^{i\theta},$$

where we used the original definitions of $\hat{a}^-$ and $\hat{a}^+$ as in eq. (568). For the modified definitions of $\hat{a}^-$ and $\hat{a}^+$ in eq. (589) in case of the square root Hamiltonian replace $\sqrt{F(n)}$ by $F(n)$. For the construction of the phase operators and phase states it is assumed in [40, 41] that the functions $F(n)$ take the values $F(n) = n\,[1+\kappa\,(n-1)]$ for $n > 0$. In each of the cases $\kappa = 0$, $\kappa > 0$ and $\kappa < 0$ $F(n)$ is a non zero sequence and consequently the series $\sum_{n=1}^{\infty} F(n)$ diverges against $+\infty$ for $\kappa \geq 0$ and against $-\infty$ for $\kappa < 0$. The same holds for $\sum_{n=1}^{\infty}\sqrt{F(n)}$ in case that $\kappa \geq 0$, $n > 0$. Therefore, the case $F(n) = \sqrt{n}$ is also contained here. The limit of $\sum_{n=1}^{\infty}\sqrt{F(n)}$ for $\kappa < 0$, $n > 0$ is undefined. Anyway, the considered phase states are the phase states constructed for the case $\kappa \geq 0$, so we do not need to bother about the case $\kappa < 0$. However, we see that the phase states are by construction no semiclassical states for $\hat{a}^-$, $\hat{a}^+$, $F(\hat{n})$ but for the phase operator $\hat{E}_\infty$. In case we define the position operator $\hat{q}$ and momentum operator $\hat{p}$ in terms of $\hat{a}^+$ and $\hat{a}^-$, in analogy to the standard case, by

$$\hat{q} := \sqrt{\frac{\hbar}{2m\omega_0}} \left(\hat{a}^+ + \hat{a}^-\right), \quad \hat{p} := i\sqrt{\frac{m\omega_0\hbar}{2}} \left(\hat{a}^+ - \hat{a}^-\right), \tag{596}$$

a calculation of their expectation values in the phase states gives

$$\langle\theta,\varphi|\hat{q}|\theta,\varphi\rangle = \sqrt{\frac{2\hbar}{m\omega_0}} \sum_{n=1}^{\infty} \sqrt{F(n)}\,\cos(\theta), \quad \langle\theta,\varphi|\hat{p}|\theta,\varphi\rangle = \sqrt{2m\omega_0\hbar} \sum_{n=1}^{\infty} \sqrt{F(n)}\,\sin(\theta). \tag{597}$$

We have a reproduction of sine and cosine, however we see that the expectation values contain for $\kappa \geq 0$, $n > 0$ the diverging series $\sum_{n=1}^{\infty} \sqrt{F(n)}$ or $\sum_{n=1}^{\infty} F(n)$ in case that we change to the definitions in eq. (589). Especially, notice that the expectation value of $F(\hat{n})$, which corresponds to the Hamiltonian operator $\hat{H}$ in this setting, in the phase states is given by

$$\langle\theta,\varphi|\hat{H}|\theta,\varphi\rangle = \langle\theta,\varphi|F(\hat{n})|\theta,\varphi\rangle = \sum_{n=1}^{\infty} F(n) \tag{598}$$

and contains the diverging series $\sum_{n=1}^{\infty} F(n)$ which does not reproduce the classical function $F(n)$. Moreover, we work with the non-unitary phase operator $\hat{E}_\infty$ which can become problematic, if we want to give a physical interpretation to it.

This brings us to the conclusion that we can use this construction method to construct phase states for the square root of the harmonic oscillator Hamiltonian but they are very limited in their range of application and have not a physical interpretation. Also the appearance of diverging series' in the calculation of the expectation values makes them not a suitable choice for semiclassical states for the square root Hamiltonian.

17 Klauder Coherent States

In [33, 42] Klauder et al. describe a method to construct coherent states for a wide class of physical systems with discrete and continuous spectra provided that the prescription of a system in the so-called action-angle-variables is known. In principle one can obtain the action-angle-variables by canonical transformations with the help of the Hamilton-Jacobi equations. However, this might not be simple and it is not a priori clear, whether the resulting classical expressions can be lifted to the operator level or not. After a short review on the construction of Klauder coherent states, we will apply this procedure to our toy model of the square root of the harmonic oscillator Hamiltonian.

17.1 Introduction to the Construction of Klauder CS

Klauder demands three defining properties for his coherent states:

1. Continuity of Labeling: The map from the label space $\mathcal{I}$ into the Hilbert space $\mathcal{H}$ is strongly continuous, i.e. $||\ell'\rangle - \ell\rangle|| \to 0$ for $\ell' \to \ell \in \mathcal{I}$.
2. Resolution of Identity.
3. Temporal Stability in the sense that for a coherent state with a classical label ℓ we have

$$e^{-i\hat{H}t}|\ell\rangle = |\ell(t)\rangle. \tag{599}$$

4. Action Identity

$$\langle J,\gamma|\hat{H}|J,\gamma\rangle = \omega J \tag{600}$$

that will be explained in detail below.

In the easiest case Klauder considers Hamiltonian operators $\hat{H}$ with a discrete, nondegenerate spectrum, energy levels of the form $0 = E_0 < E_1 < E_2 < \dots E_n$ and energy eigenstates $|n\rangle$, $n = 0, 1, 2, 3\dots$ which are solutions of the time-independent Schrödinger equation such that

$$\hat{H}|n\rangle = E_n|n\rangle = \omega e_n|n\rangle. \tag{601}$$

For this type of systems the coherent states, which we refer to as ***Klauder coherent states***, are defined by

$$|J,\gamma\rangle := N(J)^{-1/2}\sum_{n=0}^{\infty}\frac{J^{n/2}}{\sqrt{\rho_n}}e^{-ie_n\gamma}|n\rangle \tag{602}$$

with $0 \leq J < J^* \leq \infty$, $-\infty < \gamma < \infty$ and $\{\rho_n\}$ denotes a set of positive weight factors ρ_n. For convenience he chooses $\rho_0 = 1$. According to Klauder's definition of stability the Klauder coherent states are stable under time evolution. To show this we calculate

$$e^{-i\hat{H}t}|J,\gamma\rangle = N(J)^{-1/2}\sum_{n=0}^{\infty}\frac{J^{n/2}}{\sqrt{\rho_n}}e^{-ie_n(\gamma+\omega t)}|n\rangle = |J,\gamma+\omega t\rangle. \tag{603}$$

The power of the exponential in the evolved states even contains t in a linear fashion.

Normalization is then achieved by setting

$$N(J) = \sum_{n=0}^{\infty}\frac{J^n}{\rho_n} \tag{604}$$

and $J^* := \lim\inf_{n\to\infty}[\rho_n]^{1/n}$ stands for the radius of convergence of this series.

The quantities J and γ here are the so-called ***action-angle-variables***. The temporal evolution $(J,\gamma) \to (J,\gamma+\omega t)$ is the most general solution of the equations of motion

$$\dot{J} = 0, \quad \dot{\gamma} = \omega \tag{605}$$

which arise from the classical action functional $S_{class}\,[J,\gamma,t]$

$$S_{\text{class}} = \int_t \mathrm{d}t\ (J\dot{\gamma} - \omega J) \tag{606}$$

by application of the Euler-Langrange equations. There exist other classical action functionals which lead to the same equations of motion but only S_{class} above leads to the interpretation that γ and J are (classical) canonical coordinates. We follow Klauder's proposal in [33]: "The classical action principle is just the quantum action principle applied to a restricted set of Hilbert space vectors.", where a quantity called the "***quantum action***" S_{quantum} is introduced and defined as

$$S_{\text{quantum}} := \int_t \mathrm{d}t\ \left(i\langle J,\gamma|\frac{\mathrm{d}}{\mathrm{d}t}|J,\gamma\rangle - \langle J,\gamma|\hat{H}|J,\gamma\rangle\right). \tag{607}$$

Extremization of this quantum action in terms of expectation values is related with the Schrödinger equation $i\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$, where $|\psi(t)\rangle$ is a solution of the Schrödinger equation and we set $\hbar = 1$. If we wish to identify J and γ of the coherent states $|J,\gamma\rangle$ as canonical coordinates, it is necessary to demand that

$$S_{\text{quantum}} \stackrel{!}{=} S_{\text{class}}. \tag{608}$$

This leads to the so-called ***action identity***

$$\langle J,\gamma|\hat{H}|J,\gamma\rangle = \omega J \tag{609}$$

and $\langle J,\gamma|\mathrm{d}|J,\gamma\rangle = J\mathrm{d}\gamma$.

Since for the construction of Klauder coherent states we need to find the canonical transformation from the position q and momentum p variables to the action J and angle γ variables, which by definition fulfill the equations of motion in eq. (605), it is not possible to compare the solutions to the equations of motion for q and p with the expectation values of their corresponding operators in the Klauder coherent states directly. Moreover, it is a priori not clear whether the action-angle-variables can be quantized in case one wants to calculate their expectation values in the Klauder coherent states.

With the help of the action identity we can fix the positive weight factors ρ_n uniquely. The positive weight factors ρ_n are then calculated from, compare [33, 42],

$$\rho_n = \prod_{l=1}^{n} e_l. \tag{610}$$

17.2 Modified Klauder CS for the Square Root Hamiltonian

For our toy model of the one-dimensional square root of the time-independent harmonic oscillator Hamiltonian operator, we have

$$\hat{H}_{\text{sqrt}} = \sqrt{\omega_0 \hat{n}}, \tag{611}$$

where we set $\hbar = 1$ and neglect the constant $\frac{1}{2}$ term. The eigenvalue equation for the number operator eigenstates $|n\rangle$ is given by

$$\hat{H}_{\text{sqrt}}|n\rangle = E_n|n\rangle = \sqrt{\omega_0}\sqrt{\hat{n}}|n\rangle = \sqrt{\omega_0}e_n|n\rangle. \tag{612}$$

and the classical action functional for the square root Hamiltonian reads

$$S_{class} = \int\limits_t \mathrm{d}t\ \left(J\dot{\gamma} - \sqrt{\omega_0}J\right). \tag{613}$$

From the Euler-Lagrange equations we then obtain the equations of motion, namely

$$\dot{\gamma} = \sqrt{\omega_0}, \quad \dot{J} = 0. \tag{614}$$

So to be in accordance with the classical equations of motion for this system, we consider the modified action identity

$${}_{\text{sqrt}}\langle J,\gamma|\hat{H}|J,\gamma\rangle_{\text{sqrt}} = \sqrt{\omega_0}J. \tag{615}$$

Furthermore we choose $e_n = \sqrt{n}$. Making this choice the modified Klauder like coherent states for the square root Hamiltonian are given by

$$|J,\gamma\rangle_{\mathrm{sqrt}} := N(J)^{-1/2} \sum_{n=0}^{\infty} \frac{J^{n/2}}{\sqrt{\rho_n}} e^{-i\sqrt{n}\gamma} |n\rangle \tag{616}$$

with normalization factor $N(J) = \sum_{n=0}^{\infty} \frac{J^n}{\rho_n}$. The time evolution with respect to $\hat{H}_{\mathrm{sqrt}}$ becomes

$$e^{-i\hat{H}_{\mathrm{sqrt}}t}|J,\gamma\rangle_{\mathrm{sqrt}} = e^{-i\sqrt{\omega_0 \hat{n}}t}|J,\gamma\rangle_{\mathrm{sqrt}} = N(J)^{-1/2} \sum_{n=0}^{\infty} \frac{J^{n/2}}{\sqrt{\rho_n}} e^{-i\sqrt{n}(\gamma+\sqrt{\omega_0}t)}|n\rangle = |J,\gamma+\sqrt{\omega_0}t\rangle_{\mathrm{sqrt}}. \tag{617}$$

To determine the positive weight factors ρ_n, we calculate ${}_{\mathrm{sqrt}}\langle J,\gamma|\hat{H}|J,\gamma\rangle_{\mathrm{sqrt}}$ and use the modified action identity which leads to

$$\begin{aligned}
{}_{\mathrm{sqrt}}\langle J,\gamma|\hat{H}_{\mathrm{sqrt}}|J,\gamma\rangle_{\mathrm{sqrt}} &= N(J)^{-1} \sum_{m=0}^{\infty}\sum_{m=0}^{\infty} \langle m| \frac{J^{m/2}}{\sqrt{\rho_m}} \frac{J^{n/2}}{\sqrt{\rho_n}} e^{i\left(\sqrt{m}-\sqrt{n}\right)\gamma} \sqrt{\omega_0}\sqrt{n}|n\rangle \\
&= \sqrt{\omega_0} N(J)^{-1} \sum_{n=0}^{\infty} \frac{J^n}{\rho_n}\sqrt{n} \\
&\stackrel{!}{=} \sqrt{\omega_0} J = \sqrt{\omega_0} J 1 = \sqrt{\omega_0} J N(J)^{-1} N(J) \\
&= \sqrt{\omega_0} N(J)^{-1} J \sum_{n=0}^{\infty} \frac{J^n}{\rho_n} = \sqrt{\omega_0} N(J)^{-1} \sum_{n=0}^{\infty} \frac{J^{n+1}}{\rho_n}
\end{aligned} \tag{618}$$

A further comparison of line two with line four in eq. (618) yields the identity

$$\begin{aligned}
&\sum_{n=0}^{\infty} \frac{J^n\sqrt{n}}{\rho_n} \stackrel{\sqrt{0}=0}{=} \sum_{n=1}^{\infty} \frac{J^n\sqrt{n}}{\rho_n} \\
&= J\sum_{n=0}^{\infty} \frac{J^n}{\rho_n} = \sum_{n=0}^{\infty} \frac{\rho_{n+1}}{\rho_{n+1}} \frac{J^{n+1}}{\rho_n} = \sum_{n=0}^{\infty} \frac{\rho_{n+1}}{\rho_n} \frac{J^{n+1}}{\rho_{n+1}} \stackrel{n+1\to n}{=} \sum_{n=1}^{\infty} \frac{\rho_n}{\rho_{n-1}} \frac{J^n}{\rho_n}
\end{aligned} \tag{619}$$

which can only be satisfied for

$$\frac{\sqrt{n}}{\rho_n} = \frac{e_n}{\rho_n} = \frac{1}{\rho_{n-1}} \Leftrightarrow \rho_n = \sqrt{n}\rho_{n-1},\ \forall n \geq 1. \tag{620}$$

Therefore ρ_n becomes, for $\rho_0 = 1$

$$\rho_n = \prod_{\ell=1}^{n} \sqrt{\ell} = \sqrt{n!}. \tag{621}$$

Notice that this does not work for $e_n = \sqrt{n+1/2}$, since then $e_0 = \sqrt{1/2} \neq 0$ which we used explicitly to calculate the weight factors ρ_n. Finally, the modified Klauder coherent states can be expressed as

$$|J,\gamma\rangle_{\mathrm{sqrt}} = N(J)^{-1/2} \sum_{n=0}^{\infty} \frac{J^{n/2}}{\sqrt{\sqrt{n!}}} e^{-i\sqrt{n}\gamma}|n\rangle. \tag{622}$$

A couple of remarks are in order:

- The series in ${}_{\text{sqrt}}\langle J,\gamma|J,\gamma\rangle_{\text{sqrt}} = \sum_{n=0}^{\infty} \frac{J^n}{\sqrt{n!}}$ needs to converge, otherwise the states will not be normalizable, compare the discussion in [33, 42]. For the case that the series converges, we then choose the normalization factor to be $N(J) = \sum_{n=0}^{\infty} \frac{J^n}{\sqrt{n!}}$.

- To show the resolution of identity, see [33, 42], Klauder et al. assume that there exists a non-negative weight function $\rho(u)$ with $\rho(u) \geq 0$, $0 \leq u < U \leq \infty$ which satisfies

$$\rho_n = \int_0^U \mathrm{d}u\, u^n \rho(u), \quad \rho_0 = 1.$$

For U equal to the radius of convergence of the series occurring in the definition of the Klauder coherent states in eq.(602), that is $U = J^* = \lim\inf_{n\to\infty}[\rho_n]^{1/n}$, this becomes

$$\rho_n = \int_0^U \mathrm{d}J\, J^n \rho(J).$$

Therefore, ρ_n is the n-th momentum of a given distribution. To determine $\rho(J)$ from a given ρ_n is called a Stieltjes momentum problem. In our case we have $\rho_n = \sqrt{n!}$ and it is not sure whether there exists a solution.

So we see that it is difficult to use Klauder coherent states as semiclassical states for the square root Hamiltonian.

Let us close this section with a short remark on the connection between Klauder coherent states and phase states. In the phase space operator approach we have for $\hat{H}_{\text{sqrt}} = \sqrt{\hat{n}}$ the states

$$|\theta,\varphi\rangle = \sum_{n=0}^{\infty} e^{in\theta} e^{-i\sqrt{n}\varphi}|n\rangle \tag{623}$$

defined on the unit circle and not normalized. The modified Klauder coherent states are

$$|J,\gamma\rangle \equiv N(J)^{-1/2} \sum_{n=0}^{\infty} \frac{J^{n/2}}{\sqrt{\rho_n}} e^{-i\sqrt{n}\gamma}|n\rangle \tag{624}$$

From a naive point of view we can identify them by setting $\varphi = \gamma$ and taking $N(J)^{-1/2}$ also as a prefactor for the states $|\theta,\varphi\rangle$, choose $J^{1/2} = |z|e^{i\theta}\sqrt{\rho_n}$ for $z \in \mathbb{C}$ and set $|z| = 1$ to be on the unit circle. For comparison, for the time-independent harmonic oscillator we have $J^{1/2} = |z|$.

18 Complexifier Coherent States

In this section we summarize the basic construction and some properties of complexifier coherent states, since they were intensively used in semiclassical perturbation theory in part IV, are obtained from a general construction principle [43, 44, 45, 46] and allow a general discussion of their stability behaviour under time evolution [31].

Let $(\mathcal{M},\omega)$ be a symplectic manifold with strong symplectic structure ω. Remember that a ***symplectic structure*** ω is a non-degenerate, closed two form ($\mathrm{d}\omega = 0$) and a symplectic manifold is the tuple $(\mathcal{M},\omega)$. Tranformations which preserve the symplectic structure ω constitute the ***symplectic group***, in physics better known as ***canonical transformations***. The ***Liouville***

measure is the measure that is invariant under transformations of the symplectic group. Due to a theorem by Darboux, see for example [9], for a symplectic manifold in each neighbourhood of a point $p \in \mathcal{M}$ one can locally find so-called canonical coordinates $(x^\mu)_{\mu=1}^{2m} = (q^a, p_a)_{a=1}^m$ such that $\omega = dp_a \wedge dq^a$. Further, assume that $\mathcal{M}$ is the cotangent bundle of a configuration space $\mathcal{C}$ which is supposed to be a real Lagrangian submanifold, that is $\mathcal{M} := T^*\mathcal{C}$. More concretely we will later choose the classical configuration space $\mathcal{C}$ to be a compact Lie group G, then the corresponding classical phase space is the cotangential bundle of G subject to the isomorphisms

$$\mathcal{M} = T^*G \simeq G \times \mathbb{R}^{\dim G} \simeq G^{\mathbb{C}}, \tag{625}$$

where $G^{\mathbb{C}}$ is the complexification of G that is generated by the complexification of the Lie algebra $\mathfrak{g}$ of G, $\mathfrak{g} \otimes \mathbb{C}$.

According to [9] we can give the following definition of a complexifier:

Definition [9]: Complexifier 18.1. *A complexifier is a positive definite function C on $\mathcal{M}$ with the dimension of an action wich is smooth almost everywhere with respect to the Liouville measure induced from ω and whose Hamiltonian vector field is everywhere non-vanishing on the configuration space $\mathcal{C}$. Moreover, for each point $q \in \mathcal{C}$ the function $p \mapsto C_q(p) = C(q,p)$ grows stronger than linearly with $||p||_q$, where p is a local momentum coordinate and $||.||_q$ is a suitable norm on $T^*_q(\mathcal{C})$.*

Denote by q the local coordinates of the configuration space $\mathcal{C}$, then we can define local complex coordinates of $\mathcal{M}$ by

$$z(m) := \sum_{n=0}^{\infty} \frac{i^n}{n!} \{q, C\}_{(n)}(m) \tag{626}$$

with the iterated Poisson bracket $\{q,C\}_{(0)} = q$, $\{q,C\}_{(n+1)} = \{\{q,C\}_{(n)}, C\}$, $n \in \mathbb{N}_0$ for the convention $\{p,q\} = 1$ provided that z and $\bar{z}$ are invertible for $m := (q,p)$, where p are the momentum coordinates of $\mathcal{M}$.

According to the definition of the Lie derivative $\pounds$ and the Hamiltonian vector field χ_C of the complexifier C we can also write eq. (626) as

$$z = e^{-\pounds_{\chi_C}} q = \left(\left[\varphi^t_{\chi_C}\right]^* \right)_{t=-i}, \tag{627}$$

where $\left[\varphi^t_{\chi_C}\right]^*$ is the pull-back of the one-parameter family $\varphi^t_{\chi_C}$ of symplectomorphisms (canonical transformations), i.e. diffeomorphisms that preserve the symplectic structure, generated by χ_C. From this formulation we can read of that eq. (626) is an analytic extension to imaginary values of the one-parameter family $\varphi^t_{\chi_C}$. Notice that we analytically continue to the negative imaginary axis which is why positivity of C is required. The complexifier function C provides an explicit diffeomorphism from $\mathcal{M} = T^*\mathcal{C}$ to $\mathcal{C}^{\mathbb{C}}$, $m \mapsto z(m)$ such that the element $z(m) \in \mathcal{C}^{\mathbb{C}}$ carries a physical interpretation as a classical point in $\mathcal{M}$. This is where the name complexifier comes from and we see that we can consider $\mathcal{M}$ either as a symplectic or a complex manifold.

To ease the process of finding a representation, we assume that the Hilbert space $\mathcal{H}$ can be represented as a space of square integrable functions on $\mathcal{C}$ or if necessary a distributional extension $\bar{\mathcal{C}}$ thereof with respect to a positive, faithful (i.e. injective), probability measure μ i.e. $\mathcal{H} = L^2(\bar{\mathcal{C}}, \mathrm{d}\mu)$ or $\mathcal{H} = L^2(\bar{\mathcal{C}}, \mathrm{d}\mu)$ respectively. In case of a compact Lie group G, we know that G is associated with the Hilbert space $L^2(G, \mathrm{d}\mu_H)$ of square integrable functions over G with respect to the normalized Haar measure $\mathrm{d}\mu_H$.

Due to the positivity of C in the classical theory, we want to carry this property over to the quantum theory by quantizing the complexifier C so that it becomes a positive definite, self-adjoint operator. Quantization then leads to

$$\hat{z}(m) = \sum_0^\infty \frac{i^n}{n!} \frac{\left[\hat{q}, \hat{C}\right]_{(n)}}{(i\hbar)^n}(m) = e^{-\frac{\hat{C}}{\hbar}} \hat{q} e^{\frac{\hat{C}}{\hbar}} \tag{628}$$

with $\left[\hat{q}, \hat{C}\right]_{(0)} = \hat{q}$, $\left[\hat{q}, \hat{C}\right]_{(n+1)} = \left[\left[\hat{q}, \hat{C}\right]_{(n)}, \hat{C}\right]$. The division by $\hbar$ makes $\frac{\hat{C}}{\hbar}$ dimensionless. Now we introduce the δ-distribution with respect to the masure μ by $q \mapsto \delta_{q'}(q) = \delta(q', q)$ with support at $q' = q$. The δ-distribution $\delta_{q'}$ is not square integrable with respect to μ. However, in case we apply $e^{-\frac{\hat{C}}{\hbar}}$ to it and define the state

$$\psi_{q'}(q) := e^{-\frac{\hat{C}}{\hbar}} \delta_{q'}(q) \tag{629}$$

$\psi_{q'}$ has a chance to be an element of the Hilbert space $\mathcal{H}$, since $e^{-\frac{\hat{C}}{\hbar}}$ acts as a kind of smoothing operator by its positivity and non trivial dependence on momenta which become derivative operators in the quantum theory. In case we can analytically extend q' in eq. (629) to complex values $z(m) \in \mathcal{M}$ the ***complexifier coherent states*** are defined by

$$\psi_m(q) := \left[\psi_{q'}(q)\right]_{q' \to z(m)} = \left[e^{-\frac{\hat{C}}{\hbar}} \delta_{q'}(q)\right]_{q' \to z(m)}. \tag{630}$$

If $\psi_m(q)$ is a square integrable function with respect to μ, it will be an eigenfunction of the operator $\hat{z}(m)$ with eigenvalue $z(m)$ because

$$\hat{z}(m)\psi_m = \left[e^{-\frac{\hat{C}}{\hbar}} \hat{q} \delta_{q'}(q)\right]_{q' \to z(m)} = \left[q' e^{-\frac{\hat{C}}{\hbar}} \delta_{q'}(q)\right]_{q' \to z(m)} = z(m)\psi_m. \tag{631}$$

Since this is one option to define a coherent state, we will refer to $\hat{z}(m)$ as ***annihilation operator***. For our compact Lie group G this translates to

$$\psi_g^t(h) := \left(e^{\frac{t}{2}\triangle} \delta_{h'}(h)\right)\Big|_{h' \to g}. \tag{632}$$

Here $\triangle$ denotes the spectrum of $\hat{C}$, $t \propto \hbar$ is the dimensionless classicality parameter, $\delta(h)_{h'}$ is the delta distribution on G with respect to $\mathrm{d}\mu_H$, centered around $h' \in G$ and $h' \to z$ is the analytic continuation from $h' \in G$ to $g \in G^{\mathbb{C}}$. The spectrum $\triangle$ of $\hat{C}$ has to be bounded from below and has to grow such that the damping caused by the application of $e^{-\frac{\hat{C}}{\hbar}}$ to $\delta_{h'}$ decreases faster than exponentially in order to give an entire analytic expression for ψ_g^t.

In order to make sure that possibly occurring fluctuations do come out finite, we usually work with ***graph dependent complexifier coherent states***, also denoted as ***cutoff states***, which are elements of the gauge invariant Hilbert space $\mathcal{H}_{\text{kin}}$. For a given graph γ, consider all of his subgraphs $\gamma' \subset \gamma$ which are generated from γ by the removal of edges $e \subset \gamma$. Then a graph dependent δ-distribution is defined by

$$\delta_{h',\gamma}(h) := \sum_{\gamma' \subset \gamma} \sum_{s;\gamma(s)} T_s(h') \overline{T_s(h)}. \tag{633}$$

In part IV we also mentioned the measure $\mathrm{d}\nu_t(g)$ in the context of the resolution of identity for the complexifier coherent states which is included in the following Lemma:

Lemma 4.1 [44]: Measure $\nu_t(g)$ 18.2. *The* ***measure*** ν_t *underlying the* ***Coherent State Transform*** $\hat{U}_t$ *is defined by*

$$\hat{U}_t : L_2(G, \mathrm{d}\mu_H) \to \mathcal{H}L_2(G^{\mathbb{C}}, \mathrm{d}\nu_t); \quad f \mapsto \left(\hat{U}_t f\right)(g) := \langle \bar{\psi}^t_g, f \rangle, \tag{634}$$

where $L_2(G, \mathrm{d}\mu_H)$ is the Hilbert space of square integrable functions over G and $\mathcal{H}L_2$ is the Hilbert space of square integrable holomorphic functions over the complexification $G^{\mathbb{C}}$ of G, is for the group $G = \mathrm{SU}(2)$ given by

$$\mathrm{d}\nu_t(g) := \mathrm{d}\mu_H(u)\mathrm{d}\sigma_t(H) := \mathrm{d}\mu_H(u) \left[\frac{2\sqrt{2}e^{-t/4}}{(2\pi t)^{3/2}} \frac{\sinh(p)}{p} e^{-\frac{p^2}{t}} \mathrm{d}^3 p\right] := \nu_t(g)\mathrm{d}\Omega, \tag{635}$$

where $g = Hu$ is the polar decomposition of a group element g, d^3p is the standard Lebesgue measure on $\mathbb{R}^3$, $\mathrm{d}\mu_H(u)$ is the Haar measure on $\mathrm{SU}(2)$ and $\mathrm{d}\Omega = \mathrm{d}\mu_H(u)\mathrm{d}^3p$ is the Liouville measure on the cotangent bundle T^*G.

In [31] for a complexifier coherent state $|\psi_{z(t_0)}\rangle$ at a given fixed time parameter t_0 and the time evolution operator $\hat{U}(t, t_0) = \exp(i\hat{H}(t - t_0))$, $\forall t \in \mathbb{R}^+$, the stability criterion

$$\hat{U}(t, t_0)|\psi_{z(t_0)}\rangle = e^{i\lambda(t)}|\psi_{z(t)}\rangle \tag{636}$$

was introduced. Here $\exp(i\lambda(t))$ is a phase factor, with $\lambda(t)$ being a real valued function.

This stability criterion leads to the following theorem which was proven in [31].

Theorem [31]: Stability Annihilation Operator Condition 18.3. *Suppose the set of complexifier coherent states $\mathcal{S}_{t_0} := \{\psi_{z(m(t_0))}|m(t_0) \in \mathcal{M}\}$ is over-complete and stable and the time-evolution operator $\hat{U}(t, t_0)$ is unitary, then*

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{z}_j(t_0) = i f_j(\hat{z}_1, \ldots, \hat{z}_f) \quad \forall j = 1, \ldots, f, \tag{637}$$

where $f_j(\hat{z}_1, \ldots, \hat{z}_f)$ is a function which only depends on annihilation operators as given in eq. (631) and f denotes the number of degrees of freedom of the physical system in question. On the other hand, if eq. (637) holds at t_0 then there exists an $\epsilon > 0$ such that $\mathcal{S}_t := \{\psi_{z(m(t))}|m(t) \in \mathcal{M}\}$ is stable with respect to $\hat{U}(t, t_0)$ for all $|t_0 - t| < \epsilon$.

The stability criterion given in eq. (636) will also guide our stability discussion in section 21 because it is a quite general one as will be explained later on.

19 The Algebraic Construction

The methods for the construction of Klauder and Complexifier coherent states discussed in sections 17 and 18 can already be applied to find semiclassical states for a variety of physical systems but depend on finding action-angle-variables or a complexifier which needs to be quantizable. Now we want to come to the algebraic construction method for coherent states which takes as a starting point the algebra of an already quantized system. The algebraic construction can in principal be applied to all physical systems as long as one is able to determine the so-called ***spectrum generating algebra (SGA)***. To determine the SGA can be a hard task and will be discussed in detail in section 20. Like the complexifier method was inspired by the construction of the harmonic oscillator coherent states by finding an eigenstate of the annihilation operator which then is the coherent state. The algebraic construction is inspired by the application of the displacement operator to the ground state to create a coherent state. In this section we explain the components we need to construct a coherent state in the algebraic framework.

The construction of coherent states associated with an arbitrary Lie group G goes back to concepts introduced by Barut and Giradello [48], Rasetti [51] and Perelomov [49, 50]. For convenience we collect the definitions for mentioned Lie group and Lie algebra properties below. To construct a coherent state for a given Lie group G we need the following ingredients:

1. The ***homogeneous space*** $M = G/h$, where $h \subseteq G$ denotes the normal ***stability subgroup*** of G.
2. Existence of a ***cyclic vector*** $|\Omega\rangle$ in the Hilbert space $\mathcal{H}$, for a definition see 2.2.2, where cyclic in this context implies that $|\Omega\rangle$ stays an element of the Hilbert space if one acts with a group element on it.
3. An ***irreducible unitary representation*** $U(g)$ for a group element $g \in G$.

The existence of a fixed cyclic vector $|\Omega\rangle$ is guaranteed if G is either a non-compact connected, real semisimple Lie group with a finite center or it is solvable [61].

Also when G is compact and semisimple a cyclic vector $|\Omega\rangle$ exists and is given by the vector $|\Omega\rangle \in \mathcal{H}$ satisfying $U(h)|\Omega\rangle = e^{\lambda}(h)|\Omega\rangle$. So the cyclic vector is invariant under the action of the stability subgroup, except from a phase factor [61].

The coherent states $|\phi_0\rangle$ are then obtained from

$$|\phi_0\rangle := \exp(-i\alpha(g))U(g)|\Omega\rangle \tag{638}$$

with $\alpha : G \to \mathbb{R}$. For mathematical definitions see for example [110, 148, 149] and below. Many applications of this methods for example to compact and non-compact semisimple Lie groups, the Galilei group and the Poincaré group can be found in [52]. For our convenience we recall here some definitions of the properties of Lie algebras and Lie groups:

Definition [148, 149]: Compact Lie Group 19.0.1. *Each Lie group G is also a topological space. Therefore, a Lie group G is **compact** if the underlying topological space is compact. A topological space T is called compact if each of its open covers has a finite subcover. That is for every collection $\mathcal{O}$ of open subsets of X such that*

$$X = \bigcup_{x \in \mathcal{O}} x$$

there is a finite subset F of $\mathcal{O}$ such that

$$X = \bigcup_{x \in F} x.$$

Definition [148, 149]: Connected Lie Group 19.0.2. *Each Lie group G is also a topological space. Therefore, a Lie group G is **connected** if the underlying topological space is connected. A topological space is a connected space if it cannot be represented as the union of two or more disjoint non-empty open subsets.*

Definition [110]: Semisimple Lie algebra 19.0.3. *A Lie algebra $\mathfrak{g}$ is semisimple if it is a direct sum of simple Lie algebras, i.e. non-abelian Lie algebras $\mathfrak{g}$ whose only ideals are $\{0\}$ and $\mathfrak{g}$ itself.*

Definition [55]: Ideal 19.0.4. *Consider a Lie algebra $\mathfrak{g}$ and its subalgebra $\mathfrak{g}'$, that is $\mathfrak{g}' \subset \mathfrak{g}$, with elements $X_a \in \mathfrak{g}$ and $Y_b \in \mathfrak{g}'$. Since $\mathfrak{g}'$ is a subalgebra of $\mathfrak{g}$, it satisfies*

$$[Y_b, Y_c] = c'^{d}_{bc} Y_d \tag{639}$$

with structure constants c'^{d}_{bc}. If in addition the relation

$$[Y_b, X_c] = c^{d}_{bc} Y_d \tag{640}$$

*is satisfied, then $\mathfrak{g}'$ is called an **ideal** or invariant subalgebra of $\mathfrak{g}$.*

Definition[149]: Semisimple Lie Group 19.0.5. *A Lie group is semisimple if it has no non-trivial connected, normal, abelian subgroups. This is equivalent for the Lie group to have a semisimple Lie algebra.*

Definition [149]: Normal Subgroup 19.0.6. *A subgroup H of a group G is normal in G if and only if $g \circ H = H \circ g$ for all g in G; i.e., the sets of left and right cosets coincide. Normal subgroups (and only normal subgroups) can be used to construct quotient groups from a given group.*

Definition [149]: Center 19.0.7. *A **center** C is a special subgroup of a group G whose group elements commute with all elements of G, i.e.*

$$C := \{c \in G | c \circ G = G \circ c\}.$$

The elements c of C are denoted as invariant elements.

Definition [110]: Solvable Lie Algebra 19.0.8. *A Lie algebra $\mathfrak{g}$ is **solvable** if its derived series terminates in the zero subalgebra. The **derived series** is the sequence of subalgebras*

$$\mathfrak{g} \geq [\mathfrak{g}, \mathfrak{g}] \geq [[\mathfrak{g}, \mathfrak{g}], [\mathfrak{g}, \mathfrak{g}]] \geq [[[\mathfrak{g}, \mathfrak{g}], [\mathfrak{g}, \mathfrak{g}]], [[\mathfrak{g}, \mathfrak{g}], [\mathfrak{g}, \mathfrak{g}]]] \geq \dots.$$

Definition [149]: Solvable Group 19.0.9. *A group G is called solvable if it has a subnormal series whose factor groups (quotient groups) are all abelian, that is, if there are subgroups $\{1\} = G_0 < G_1 < \ldots < G_k = G$ such that G_{j1} is normal in G_j, and G_j/G_{j1} is an abelian group, for $j = 1, 2, \ldots, k$. This is equivalent for the Lie group to have a solvable Lie algebra.*

Table 1 below summarizes some properties of Lie groups and their corresponding Lie algebras. By $G(p,q)$ we mean an indefinite group with $p+q = N \in \mathbb{N}$ and $p \geq q \geq 1$. Due to the generation of a Lie group from a Lie algebra by the exponential map, the reality, solvability and simplicity properties carry over to the algebra or vice versa. A semisimple Lie algebra is never solvable, see [150] and a nilpotent Lie algebra or an abelian Lie group are always solvable, see [110].

In the following we identify $U(g)$ with the exponential of linear combinations of (representations of) Lie algebra elements $\hat{G}_i$, which usually gives rise to the group, and apply it to a vacuum state in physical terms or more general a cyclic vector Ω. Here the θ_i are constants $\in \mathbb{C}$ or complex valued functions which might label the classical phase space with $i \in \mathcal{I}$ and $\mathcal{I}$ is an arbitrary index set. Subsequently, the coherent state is then defined by

$$|\phi_0\rangle := e^{\sum_i \theta_i \hat{G}_i} |\Omega\rangle, \tag{641}$$

where we neglect phase factors.

Table 1: Properties of Lie groups and corresponding Lie algebras

Lie group	compact	connected	semisimple	solvable	real	Lie algebra
$O(N)$	y	n	y, $N \geq 3$	n, $N \geq 3$	y	$so(N)$
$O(N,\mathbb{C})$	n, $N > 1$	n	y, $N \geq 3$	n, $N \geq 3$	n	$so(N,\mathbb{C})$
$O(p,q)$	n	n	y, $p+q \geq 3$	n, $p+q \geq 3$	y	$so(p,q)$
$SO(N)$	y	y, s $N=1$	y, $N \geq 3$	n, $N \geq 3$	y	$so(N)$
$SO(N,\mathbb{C})$	n, $N > 1$	y	y, $N \geq 3$	n, $N \geq 3$	n	$so(N,\mathbb{C})$
$SO(p,q)$	n	n	y, $p+q \geq 3$	n, $p+q \geq 3$	y	$so(p,q)$
$U(N)$	y	y	n	y	y	$u(N)$
$U(p,q)$	n	n	n	y	y	$u(p,q)$
$SU(N)$	y	y, s	y, $N \geq 2$	n, $N \geq 2$	y	$su(N)$
$SU(p,q)$	n	n	y, $p+q \geq 2$	n, $p+q \geq 2$	y	$su(p,q)$
$GL(N,\mathbb{R})$	n	n	n	n, $N \geq 2$	y	$gl(N,\mathbb{R})$
$GL(N,\mathbb{C})$	n	y	n	n, $N \geq 2$	n	$gl(N,\mathbb{C})$
$WH(N,\mathbb{R})$	locally	y, s	n	y	y	$wh(N,\mathbb{R})$

The small letters stand for n=no, y=yes and s=simply connected. Here $WH(N,\mathbb{R})$ denotes the (Weyl)-Heisenberg group.

20 Spectrum Generating Algebras

In this section we have a closer look at the definition of the SGA as well as the definitions of the symmetry algebra (SA) and the dynamical group and we introduce some methods to find a SGA.

20.1 Definitions and Results for the SGA

To the best of our knowledge Dothan is the first who introduces in [53] the notion of finite dimensional ***spectrum generating algebras (SGAs)*** with a short comment at the end of his article how the framework can be extended to the infinite dimensional case. The SGA is the algebraic description of a physical system. The idea of the SGA arises from the observation that in certain physical problems the energy eigenstates with **different energies** form a basis for a single unitary irreducible representation of a Lie algebra. Similar to the invariant approach in [151, 152, 153] Dothan claims in [53] that the generators of a spectrum generating algebra (SGA) are constants of motion, maybe explicitly time-dependent. He first defines the ***symmetry algebra (SA)*** as a subalgebra of the SGA and then introduces the SGA as a generalization of the SA.

Definition [53]: Symmetry Algebra (SA) by Dothan 20.1.1. *The SA consists of Hermitian operators without explicit time dependence that satisfy the following conditions:*

a) They commute with the Hamiltonian operator. $\Rightarrow$ Constants of motion.

b) They form a Lie algebra under commutations.

c) The SA is maximal, that is for any energy eigenvalue the space of all degenerate states is irreducible under the SA.

d) The SA is minimal, that is the SA does not contain a proper subalgebra with the same properties.

To define the SGA one now wants to generalize the defining properties of the SA such that the SA is a subalgebra of the SGA and all the energy eigenfunctions form a single unitary irreducible representation of the SGA. The generalization of the last three properties b) to d) is obvious but the generalization of property a) is more involved. To archive at this generalization Dothan uses two results. The first result is from Malkin and Man'ko [154]. They observed that if $\psi(q;t)$ is any solution of the time-dependent Schrödinger equation

$$\left[i\frac{\partial}{\partial t} - \hat{H}(p,q)\right]\psi(q;t) = 0, \tag{642}$$

where here and in the following we set $\hbar = 1$, then $\hat{G}(p,q;t)\psi(q;t)$ will also be a solution of the time-dependent Schrödinger equation in case that $\hat{G}$ satisfies the condition

$$i\frac{\partial \hat{G}}{\partial t} - \left[\hat{H},\hat{G}\right] = 0. \tag{643}$$

Therefore, $\hat{G}$ is a constant of motion but it is now allowed to have an explicit time dependence. If $\hat{G}$ is a Hermitian operator which satisfies eq. (643) and if $\psi(q;t)$ is a normalized solution of the time-dependent Schrödinger eq. (642), then $\exp(ia\hat{G})\psi(q;t)$ is also a normalized solution of the time-dependent Schrödinger eq. (642) for $a \in \mathbb{R}$, independent of p, q and t. This means that $\hat{G}$ can be exponentiated to form a one-parameter group of transformations.

The second remark that Dothan uses comes from Lipkin [155] it states that if $\hat{G}$ satisfies eq. (643) and has non-trivial time dependence , that is $\frac{\partial \hat{G}}{\partial t} \neq 0$, then $\hat{G}\psi$ is a linear combination of eigenstates of $\hat{H}$ with different energies. This means that $\hat{G}$ *generates the spectrum of* $\hat{H}$.

Both insights lead Dothan to the proposal to adopt eq. (643) as a generalization of condition a). In search for operators that do not commute with the Hamiltonian operator $\hat{H}$ the condition in eq. (643) will give us some guidance in the vast pool of options.

We remark that it is not clear that a finite dimensional SGA exists at all. However, Dothan noticed that for a system with a finite number of degrees of freedom the states are labeled by a finite number of quantum numbers. Therefore, a finite dimensional SGA should characterize such a system completely. Using these results Dothan arrived at the following definition for the SGA.

Definition [53]: Spectrum Generating Algebra (SGA) by Dothan 20.1.2. *The SGA* $\mathfrak{S}$ *of a physical system is a Lie algebra consisting of the set of all Hermitian operators (generators)* $\hat{G}_i\,(p,q;t)$ *which fulfill eq.* (643)*, that is*

$$\mathfrak{S} = \left\{\hat{G}_i; i\frac{\partial}{\partial t}\hat{G}_i - \left[\hat{H},\hat{G}_i\right] = 0\right\}, \tag{644}$$

where the Hamiltonian operator is not explicitly time-dependent ($\frac{\partial \hat{H}}{\partial t} = 0$)*.*

The SGA $\mathfrak{S}$ possess as a subset the set $\mathfrak{D}$ of all Hermitian operators $L_b(p,q)$ which are time-independent and fullfill eq. (643), in signs

$$\mathfrak{D} = \left\{\hat{L}_j; \frac{\partial}{\partial t}\hat{L}_j = 0, \left[\hat{H},\hat{L}_j\right] = 0\right\}. \tag{645}$$

$\mathfrak{D}$ forms an infinite-dimensional Lie subalgebra of the Lie algebra $\mathfrak{S}$. For a system with finite degrees of freedom conditions c) and d) are expected to be sufficient to ensure the existence of a finite dimensional subalgebra $\mathfrak{D}_{fin}$ which is the SA of the problem. The choice of $\mathfrak{D}_{fin}$ is in general not unique.

A modern compendium of definitions of the SA, SGA and dynamical symmetries can be found in Iachello's book [55].

Definition [55]: Spectrum Generating Algebra (SGA) by Iachello 20.1.3. *A Lie algebra $\mathfrak{g}$ is called a spectrum generating algebra, if the Hamiltonian operator $\hat{H}$ and other operators of physical interest can be written in terms of the elements $\hat{G}_i$ of the Lie algebra $\mathfrak{g}$, i.e. $\hat{H} = f(\hat{G}_i)$ where $\hat{G}_i \in \mathfrak{g}$.*

Definition [55]: Symmetry Algebra (SA) by Iachello 20.1.4. *The symmetry algebra of a Lie algebra $\mathfrak{g}$ is the subalgebra of $\mathfrak{g}$ whose elements commute with the Hamiltonian operator.*

Definition [55]: Dynamic(al) Symmetries by Iachello 20.1.5. *One speaks about dynamic(al) symmetries in case that the Hamiltonian operator $\hat{H}$ does not contain all elements of $\mathfrak{g}$, but only those combinations which form the **Casimir operators** of a chain of algebras originating from $\mathfrak{g} \supset \mathfrak{g}' \supset \mathfrak{g}'' \supset \ldots$.*

Definition [55]: Casimir Operator 20.1.6. *An operator which commutes with all the elements of a Lie algebra $\mathfrak{g}$ is called an invariant or Casimir Operator $\hat{C}$, i.e.*

$$\left[\hat{C}, \hat{G}_i\right] = 0 \tag{646}$$

for any $\hat{G}_i \in \mathfrak{g}$. It lies in the enveloping algebra of $\mathfrak{g}$, for an explanation see section 21.4.1. The Casimir operator is called of order $p \in \mathbb{N}$, if it is build from products of p elements

$$\hat{C}_p = \sum_{i_1, i_2 \ldots, i_p} c^{i_1 i_2 \ldots i_p} \hat{G}_{i_1} \hat{G}_{i_2} \cdots \hat{G}_{i_p}. \tag{647}$$

for constants $c^{i_1 i_2 \ldots i_p}$.

For many instructive examples concerning the use of Lie algebras in physics, chains of algebras and their Casimir operators also see Iachello's book [55].

In chapter 10 of Wulfman' book [54] we find the following definition of the SGA or the spectrum generating group.

Definition [54]: Spectrum Generating Group by Wulfman 20.1.7. *Groups whose generators and/ or operators convert an energy eigenstate into sets of eigenstates, labeled by energy eigenvalues of group generators that do or do not commute with the Hamiltonian, are said to be spectrum generating.*

So the modern definitions agree with Dothan's original definition in eq. (644) with more or less details mentioned.

20.1.1 Closed Lie Algebras as SGAs

In the upcoming we repeat here the argumentation from [53] why Lie algebras are preferred SGAs. We come back to the algebra $\mathfrak{S}$ in eq. (644) and consider the unique solutions

$$\hat{q}_0 = e^{i\hat{H}t} \hat{q} e^{-i\hat{H}t} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \left[\hat{H}, \hat{q}\right]_{(n)}, \quad \hat{p}_0 = e^{i\hat{H}t} \hat{p} e^{-i\hat{H}t} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \left[\hat{H}, \hat{p}\right]_{(n)} \tag{648}$$

of eq. (643) for the initial conditions $\hat{q}_0(0) = \hat{q}$ or $\hat{p}_0(0) = \hat{p}$ with the iterated Lie bracket $\left[\hat{H}, \hat{G}\right]_{(0)} = \hat{G}$, $\left[\hat{H}, \hat{G}\right]_{(n+1)} = \left[\hat{H}, \left[\hat{H}, \hat{G}\right]_{(n)}\right]$ for $\hat{G} \in \{\hat{q}, \hat{p}\}$. For a system with f degrees of freedom they constitute a complete set of $2f$ operators so that every member of $\mathfrak{S}$ is a function $F(\hat{q}_0, \hat{p}_0)$ of $\hat{q}_0$ and $\hat{p}_0$. Now we want to construct a finite-dimensional Lie algebra out of the infinite dimensional Lie algebra of $\mathfrak{S}$. On the first view this seems to be accomplished by considering the set of operators $\{\hat{q}_0, \hat{p}_0\}$, since they satisfy the algebra

$$[\hat{q}_0, \hat{p}_0] = i\hat{\mathbb{1}}. \tag{649}$$

However, the knowledge of this algebraic structure is useless, since it does not contain any information about the dynamics of our physical system except the number of degrees of freedom.

To bring in some information about the dynamics of the physical system in consideration, we have to consider the commutators

$$\frac{1}{i}\left[\hat{H}, \hat{q}_0\right], \quad \frac{1}{i}\left[\hat{H}, \hat{p}_0\right]. \tag{650}$$

If $\hat{p}_0$, $\hat{q}_0$ and $\hat{H}$ are Hermitian operators, their commutators will again be Hermitian operators and by eq. (643) we know that they should be equal to

$$\frac{\partial \hat{q}_0}{\partial t} = \frac{1}{i}\left[\hat{H}, \hat{q}_0\right], \quad \frac{\partial \hat{p}_0}{\partial t} = \frac{1}{i}\left[\hat{H}, \hat{p}_0\right]. \tag{651}$$

Again they are members of the algebra $\mathfrak{S}$. They functionally depend on the operators $\hat{p}_0$ and $\hat{q}_0$. This dependence however is in general non-linear and the time derivatives in eq. (651) will in general yield to a number of additional generators. For the choice of a linearly independent set of generators, we will even need more and more generators to make it a closed set under commutation. So we will need to successively calculate higher time derivatives or commutators and end up in general with an infinite dimensional algebra.

To avoid the generation of more and more generators, we can introduce some additional demands on our generators. These will allow us to obtain a finite dimensional subset of $\mathfrak{S}$, denoted by $\mathfrak{S}_{fin}$, which will give rise to the finite-dimensional SGA. We demand that

1. A commutator of two elements in $\mathfrak{S}_{fin}$ is again an element in $\mathfrak{S}_{fin}$.
2. The time derivative of an element in $\mathfrak{S}_{fin}$ is again in $\mathfrak{S}_{fin}$. However, this has to be realized in a finite linear fashion.

For a Lie algebra, including the Hamiltonian operator, the conditions are both satisfied.

In a more formal way, let us consider a finite set of Hermitian operators $\hat{G}_i\left(\hat{p}, \hat{q}, t\right)$ wich in addition to eq. (643) have the properties

$$\left[\hat{G}_i\left(\hat{p}, \hat{q}, t\right), \hat{G}_j\left(\hat{p}, \hat{q}, t\right)\right] = c_{ij}^k \hat{G}_k\left(\hat{p}, \hat{q}, t\right), \tag{652}$$

$$\frac{\partial}{\partial t}\hat{G}_i\left(\hat{p}, \hat{q}, t\right) = \omega_j^k \hat{G}_k\left(\hat{p}, \hat{q}, t\right), \tag{653}$$

where $c_{ij}^k \in \mathbb{R}$ are structure constants, that is a Lie algebra. The indicated dependence of the operators $\hat{G}_i\left(\hat{p}, \hat{q}, t\right)$ on canonical variables $\hat{p}$ and $\hat{q}$ stands for the dependence on any, not necessarily canonical, set of dynamical variables. We refer to the $\omega_j^k \in \mathbb{R}$ as the ***frequency matrix elements***. First we assume that they are time-independent and commute with all generators of the SGA.

The solutions to eq. (653) according to [53] are given by

$$\hat{G}_i(p, q; t) = \left(e^{\omega t}\right)_i^j \hat{G}_j(p, q; t = 0) \tag{654}$$

with

$$e^{\omega t} = \sum_{k=1}^{s} e^{\nu_k t} \left(\sum_{\ell=1}^{r_k} t^{\ell-1} Z_{k\ell} \right), \tag{655}$$

where $Z_{k\ell}$ denote matrices which are polynomials in the matrix ω, ν_k denote the different eigenvalues of the matrix ω and r_k are their multiplicities in the minimal polynomial of the matrix ω. So the explicit time-dependence of the generators is given by a polynomial in t times an exponential function in t. We will refer to this as the ***standard time-dependence***. Particular for a **semisimple algebra the time-dependence is purely exponential**. We stress, as remarked in [53], that the t derivative of a function in the class of solutions is again a member of the class of solutions. The results related with the time evolution of the generators are in accordance with our considerations in section 21.2 concerning the discussion of stability of semiclassical states in the context of the algebraic construction.

Equation (653) contains the dynamical information about our physical system in consideration and combined with eq. (643) gives

$$\left[\hat{H}, \hat{G}_i\left(\hat{p}, \hat{q}, t\right)\right] = i\omega_j^k \hat{G}_k\left(\hat{p}, \hat{q}, t\right) \tag{656}$$

which ensures that the Hamilton operator maps the algebra into itself. It is important to notice that different physical systems can have the same algebra as in eq. (652), but eq. (656) differs due to its dynamical content.

20.1.2 Properties of the SGA

Assume that the c_{ij}^k are known. With the help of the c_{ij}^k we can determine the ω_j^k. For this purpose we remember ourselves that the structure constants of a Lie algebra satisfy the ***Jacobi identity***

$$c_{ij}^k c_{k\ell}^m + c_{j\ell}^k c_{ki}^m + c_{\ell i}^k c_{kj}^m = 0. \tag{657}$$

Moreover, for eq. (652) and eq. (653) to be mutually compatible they need to satisfy the so-called ***Bargmann type identity***, see eq. (4.26) in [156], given by

$$c_{ij}^k \omega_k^m + c_{ki}^m \omega_j^k + c_{jk}^m \omega_i^k = 0. \tag{658}$$

With this one can verify that the following expression for the frequency matrix satisfies eq. (658)

$$\omega_k^m = \beta^\ell c_{k\ell}^m, \tag{659}$$

where the β^ℓ are real, time-independent and commute with all the $\hat{G}_i$

According to [53] a Hamiltonian operator with a frequency matrix of the type in eq. (659) is referred to as a ***linear Hamiltonian operator*** and can be written as

$$\hat{H} = -\beta^i \hat{G}_i + \hat{C}, \tag{660}$$

where $\hat{C}$ commutes with all the $\hat{G}_i$. Now consider the following Lie subalgebra, called ***Augemented Symmetry Algebra***:

Definition: Augmented Symmetry Algebra (ASA) 20.1.8. *The augmented symmetry algebra is a subalgebra of the SGA whose generators commute with the Hamiltonian operators and that contains the SA.*

It follows that a linear Hamiltonian operator is a linear Casimir operator on the ASA, see definition 20.1.6. However, a linear Casmir operator exists only for a non-semisimple algebra. This leads to the conclusion that a **linear Hamiltonian possesses a non-semisimple ASA.** For more informations how to find the ASA with the help of action-angle vatiables, we refer the reader also to [53].

However, now we come to the critical point. In [53] it is then assumed that the set of c_{ij}^k defines a semisimple SGA which means that indices can be raised and lowered with the metric $g_{i\ell} = c_{ij}^k c_{\ell k}^j$. Then he shows that the only possible frequency matrices have the form

$$\omega_{km} = \beta^\ell c_{k\ell m}, \tag{661}$$

where the β^ℓ are again real, time-independent and commute with all the $\hat{G}_i$. So we have the following situation: **if the SGA is semisimple, the only possible Hamiltonians in Dothan's framework will be linear Hamiltonians** but the Augemented Symmetry Algebra, which is a Lie subalgebra of the SGA, in contradiction is non-semisiple. This shows that the closed algebra condition in eq. (653) is nice to handle but too restrictiv.

As a physical implication Dothan also proves in [53] that the formalism in its current form for a semisimple Lie algebra always gives rise to an energy spectrum of a set of harmonic oscillators, i.e. energy values of equal spacing. A counter example is the semisimple SGA for the bound states of the hydrogen atom which is $so(4,2)$ but whose energy values have no equal spacing, see for example [39]. More examples for semisimple Lie algebras are su(N) for $N \geq 2$ or so(N) for $N \geq 3$, see also section 19.

Thus, we have to relax the condition in eq. (653) or in eq. (656).

20.1.3 Enlarging the Framework

There are two possibilities to enlarge the framework by relaxing eq. (653).

1. Generate more general types of explicit time dependence by making the frequency matrix time-dependent.
2. Relax the scheme by allowing the frequency matrix to depend on physical quantities of the system in consideration as well as generators of the algebra.

One example for the second option which is motivated and explained in [53] is to allow the ω_i^j to be Hermitian functions of the generators L_k that commute with the Hamiltonian, that is $\{\omega_i^j(L_k), H\} = 0$ with $\omega_i^j = \omega_i^j(L_k)$ Hermitian. The ω_i^j can be time-independent functions of masses, coupling constants, Casimir operators of the algebra generated by the L_k and the degrees of freedom that commute with all the $G's$. As explained in [53] this leads to spectra with non-equal spacings. Notice that the Kepler problem falls into this category, compare also [157]. Consequently, as equation between operators eq. (653) is not necessarily valid.

What we learn from this section is that Lie algebras are easy to handle candidates for spectrum generating algebras, however we have to be careful to take enough generators into a account to really describe the dynamics of a physical system and not only its kinematics. On the other hand for a finite dimensional problem, we should be able to find a finite number of generators. To impose additional conditions to make the algebra finite can be tempting but have to be checked carefully in order to describe the physical properties of the system correctly.

20.2 Methods to find Spectrum Generating Algebras

We summarize the following methods to uncover spectrum generating algebras or groups, compare also [54]:

1. Factorization method by Infeld and Hall, originally [158].
   - Factoring a Hamiltonian into a product of raising and lowering operators
2. Generalized Lie theory of differential equations by Lie [157].
   - Hamilton operator commutes with the Casimir operator of his invariance group.
3. Finding symmetry generators for Hamiltonians including polynomials of operators with known energy spectrum [62].

In the beginning of this part we encountered some factorization methods where the Hamiltonian operator can be factorized in (generalized) annihilation and creation operators, see the time-independent harmonic oscillator in section 14.2, the effective Hamiltonian resulting from the inverse Thiemann identity in section 15, the generalized Weyl-Heisenberg algebra wh in section 16 and the SUSY Hamiltonians in Nieto [34] or appendix H.1. In the upcoming we will represent different methods to find a SGA for a particle in one-dimension in a potential and finally for more general systems whose Hamiltonian is a function of an operator with known energy spectrum. During the course of this section we will come to the generalized Lie theory of differential equations which actually allows to find certain dynamical symmetries known as Cartan symmetries. At the end we display a method shown in [54]. The method helps to find symmetry generators for Hamiltonian operators consisting of a polynomial in an operator whose spectrum is known. We try to apply it to the square root Hamiltonian, even though it is originally not meant for this case.

As a remark in advance, we observed that one way to find a SGA can be to calculate commutators of already known generators which is also shortly mentioned in [157] but is not a systematic method. Another option can be to use "combinations" of familiar generators as for example done in [53] to find the SGA and the SA of the free spinless particle in three dimensions. The SGA of the free spinless particle is the algebra corresponding to the Galilei group. The generators are the space translations $\vec{P}$, the velocity transformations $\vec{K}$ and the identity $\mathbb{1}$. In terms of Cartesian canonical coordinates and momenta the generators read

$$\vec{P} = \vec{p}, \ \vec{K} = m\vec{q} - \vec{p}t. \tag{662}$$

We can also obtain additional generators by

$$\vec{K} \times \vec{P} = (m\vec{q} + \vec{p}t) \times \vec{p} = m\left(\vec{q} \times \vec{p}\right) = m\vec{J}, \tag{663}$$

where $\vec{J} := \vec{q} \times \vec{p}$ is the generator of rotations. The enlarged SGA is now build by the generators $\vec{P}, \vec{J}, \vec{K}$ and the identity matrix $\mathbb{1}$. The commutators of their components can be found in [53] and also show that the SA is formed by the the operators $\vec{P}, \vec{J}$.

20.2.1 Symmetries of Differential Equations

In [157] discusses how one can find and use the knowledge of symmetries of differential and partial differential equations to find their or some of their solutions. A method for finding dynamical symmetries, see definition 20.1.5, for systems possessing a Lagrangian closely related to the invariants is given by Stephani in chapter 13 of his book [157]. With the given method one can determine a subclass of dynamical symmetries the so-called ***Cartan symmetries***. In general it is impossible to find all dynamical symmetries of a given differential equation, which might be related to a physical system by the equations of motion. To find the Cartan symmetries one makes a polynomial ansatz for the so-called ***first integrals*** which are functions φ depending on the time t and coordinates $q^a(t)$ that satisfy $\frac{\mathrm{d}}{\mathrm{d}t}\varphi = 0$. Let q^a be some coordinates and $\dot{q}^a$ their derivatives with respect to the time-parameter t, if $L(t, q^a(t), \dot{q}^a(t))$ is the Langrangian of a physical system characterized by

$$\mathbf{A} := \frac{\partial}{\partial t} + \dot{q}^a \frac{\partial}{\partial q^a} + \omega^a(q^k, \dot{q}^k, t)\frac{\partial}{\partial \dot{q}^a} \tag{664}$$

and if the ***generator of the Cartan symmetry*** is defined by

$$\mathbf{X} := \xi(q^k, \dot{q}^k, t)\frac{\partial}{\partial t} + \eta^a(q^k, \dot{q}^k, t)\frac{\partial}{\partial q^a} + \dot{\eta}^a(q^k, \dot{q}^k, t)\frac{\partial}{\partial \dot{q}^a} \tag{665}$$

for $a, k = 1, \ldots, N$ and $|\partial^2 L/\partial \dot{q}^a \partial \dot{q}^b| \neq 0$, there exists a first integral φ with $\mathbf{A}\varphi = 0 = \varphi\mathbf{X}$ such that

$$\frac{\partial^2 L}{\partial \dot{q}^a \partial \dot{q}^b}\left(\eta^a - \dot{q}^a \xi\right) = -\frac{\partial \varphi}{\partial \dot{q}^b} \tag{666}$$

holds. From this one can see that the method cannot be applied to constraint systems, where it is not possible to solve for the velocities v, since $v = \partial L/\partial \dot{q}^a = 0$. Vice versa if a first integral φ is given, then $(\eta^a - \dot{q}^a\xi)$ in equation (666) determines a Cartan symmetry (special dynamical symmetry) up to gauge transformations of the form $\mathbf{X}' = \mathbf{X} + \rho\mathbf{A}$. The advice given in chapter 13 of Stephani's book is if the Lagrangian is quadratic in $\dot{q}^a$, look for first integrals that are polynomials in $\dot{q}^a$ by solving $\mathbf{A}\varphi = 0$. However, for Lagrangians that contain higher powers of $\dot{q}^a$ one can try a similar ansatz. In any way it might be a good guess to look for first integrals that have a similar dependence on $\dot{q}^a$ than the Lagrangian has. This method cannot be applied to our square root Hamiltonian toy model, since it implicitly uses the assumption that we can define a Lagrange function containing only polynomials in q^a and $\dot{q}^a$.

1dim Particle in a Potential:
As an example we consider the Lagrangian for a particle in one-dimension with mass $m \neq 0$ in a non-velocity dependent potential $V(q(t))$ given by

$$L(t, q(t), \dot{q}(t)) = \frac{m}{2}\dot{q}^2 - V(q(t)), \tag{667}$$

where a dot denotes the derivative with respect to the time parameter t. An ansatz for its first integral is given by

$$\varphi = \frac{1}{2}K_{11}\dot{q}^2 + K_1\dot{q} + K, \tag{668}$$

where K_{11}, K_1 and K are functions of t and $q(t)$. The equation of motion for the one dimensional free particle in a potential $V(q(t))$ reads

$$\ddot{q} = -\frac{1}{m}\frac{\partial V(q)}{\partial q} := -\frac{1}{m}V_{,q}. \tag{669}$$

Then we can calculate the total time derivative of φ and try to find the conditions for which it becomes zero:

$$
\begin{aligned}
0 \overset{!}{=} \frac{\mathrm{d}}{\mathrm{d}t}\varphi = \frac{1}{2}K_{11,q}\dot{q}^3 + \left(\frac{1}{2}K_{11,t} + K_{1,q}\right)\dot{q}^2 \\
+ \left(K_{1,t} + K_{,q} - \frac{1}{m}V_{,q}K_{11}\right)\dot{q} \\
+ K_{,t} - \frac{1}{m}V_{,q}K_1,
\end{aligned} \tag{670}
$$

where we used that $\ddot{q} = \frac{1}{m}V_{,q}$ and a comma followed by a letter means a partial derivative with respect to the corresponding variable. Therefore, for the third order term we obtain

$$
\frac{1}{2}K_{11,x} = 0 \Rightarrow K_{11} = a(t). \tag{671}
$$

The second order terms lead to

$$
\begin{aligned}
&\frac{1}{2}K_{11,t} + K_{1,q} = 0 \Leftrightarrow K_{1,q} = -\frac{1}{2}K_{11,t} = -\frac{1}{2}a_{,t} \\
&\Rightarrow K_1 = -\frac{1}{2}a_{,t}q + b(t), \quad K_{1,t} = -\frac{1}{2}a_{,tt}q - \frac{1}{2}a_{,t}\dot{q} + b_{,t}.
\end{aligned} \tag{672}
$$

We insert the results obtained so far again in the first integral condition to determine the function K

$$
\begin{aligned}
0 \overset{!}{=} \frac{\mathrm{d}}{\mathrm{d}t}\varphi =& K_{1,t}\dot{q} + K_{,q}\dot{q} - \frac{1}{m}V_{,q}K_{11}\dot{q} + K_{,t} - \frac{1}{m}V_{,q}K_1 \\
=& -\frac{1}{2}a_{,tt}q\dot{q} - \frac{1}{2}a_{,t}\dot{q}^2 + b_{,t}\dot{q} + K_{,q}\dot{q} - \frac{1}{m}V_{,q}a\dot{q} \\
&+ K_{,t} - \frac{1}{m}V_{,q}\left(-\frac{1}{2}a_{,t}q + b\right).
\end{aligned} \tag{673}
$$

From this we can conclude that $a_{,tt}$ and $a_{,t}$ have to vanish, i.e. $a_{,t} = a_{,tt} = 0$ in order to get rid of the second order and mixed q and $\dot{q}$ terms which is the case for $a(t) = const. := c_1$ being a constant. Now the first and zero order terms become

$$
b_{,t} + K_{,q} - \frac{1}{m}V_{,q}a = 0 \Rightarrow K = -b_{,t}q + \frac{c_1}{m}V(q) + c(t) \tag{674}
$$

and with this

$$
K_{,t} - \frac{b}{m}V_{,q} = -b_{,tt}q - b_{,t}\dot{q} + \frac{\partial}{\partial t}\left(\frac{c_1}{m}V(q)\right) - \frac{b}{m}V_{,q} + c_{,t} = 0 \tag{675}
$$

which is satisfied for $b_{,t} = b_{,tt} = 0$ and $c_{,t} + \frac{\partial}{\partial t}\left(\frac{c_1}{m}V(q)\right) - \frac{b}{m}V_{,q} = 0$ which means that $b(t) = const. := c_2$ and $c(t) = \int \mathrm{d}t\frac{b}{m}V_{,q} - \frac{c_1}{m}V(q) + c_3$, where c_3 is a constant.

So the first integral is finally given by

$$
\varphi = \frac{1}{2}c_1\dot{q}^2 + c_2\dot{q} + \int \mathrm{d}t\frac{b}{m}V_{,q} + c_3. \tag{676}
$$

For the particle in a potential $V(q(t))$ we have

$$
\begin{aligned}
&\frac{\partial^2 L}{\partial\dot{q}\partial\dot{q}}\left(\eta - \dot{q}\xi\right) = -\frac{\partial\varphi}{\partial\dot{q}} \Leftrightarrow m\left(\eta - \dot{q}\xi\right) = -c_1\dot{q} - c_2 \\
&\Rightarrow \xi = \frac{a}{m}, \quad \eta = -\frac{b}{m}.
\end{aligned} \tag{677}
$$

The generator of the Problem is given by

$$X = \frac{c_1}{m}\frac{\partial}{\partial t} - \frac{c_2}{m}\frac{\partial}{\partial q} \tag{678}$$

or we can also chose for example $c_1 = 0$, $c_2 = 1$ and $c_1 = 1$, $c_2 = 0$ and write down one generator for each parameter, that is

$$X_1 = -\frac{1}{m}\frac{\partial}{\partial q}, \quad X_2 = \frac{1}{m}\frac{\partial}{\partial t}. \tag{679}$$

Assuming that the partial derivative applied to a smooth function can be interchanged, their commutator vanishes

$$[X_1, X_2] = 0. \tag{680}$$

So as long as the potential does not depend on the velocity $\dot{q}$, the generators of the Cartan symmetries are the same as for the free particle as calculated in appendix H.2. Therefore, for one-dimensional problems and potentials that only depend on q and not on $\dot{q}$ the algebra is just the Abelian o(1) algebra. This is in agreement with the definition of the degeneracy algebra for one dimensional problems in Iachello's book [55] which describes on the operator level all operators that commute giving rise to the same energy eigenvalues. For polynomials in q and $\dot{q}$ the situation changes, since for example the third order equation in $\dot{q}^3$ might be different. Also for higher dimensions one has different results for the free particle and a particle in a potential, see Stephani's book [157]. We mention that one example discussed there in detail is the three dimensional Kepler problem. In general the resuting algebra of the found generators does not need to be a Lie algebra, as explained in [157] in case of the Kepler problem.

Compare also to the example for the free particle in one dimension moving along the q-axis in [54] which has a Lie algebra generating a continuous spectrum. The generator of the Lie group in this case is

$$\hat{Q}_2 = q\frac{\partial}{\partial q} + 2t\frac{\partial}{\partial t} \tag{681}$$

with the commutation relations

$$\left[\hat{H}, \hat{Q}_2\right] = -2\hat{H}, \quad \left[i\frac{\partial}{\partial t}, \hat{Q}_2\right] = -2i\frac{\partial}{\partial t}, \tag{682}$$

where the last commutation relation follows from the time-dependent Schrödinger equation. As shown in [54] commutator relations of this form imply that $\hat{H}$ and $i\frac{\partial}{\partial t}$ have a continuous spectrum. In general there it is shown that given $\hat{Q}$ is the generator of an invariance transformation of a time-dependent Schrödinger equation and suppose that $\hat{Q}$ satisfies

$$\left[\hat{H}, \hat{Q}\right] = b\hat{H} \quad \text{and} \quad \left[\hat{Q}, i\frac{\partial}{\partial t}\right] = bi\frac{\partial}{\partial t} \tag{683}$$

with $-\infty < b < \infty$, then the corresponding physical system has a continuous spectrum.

20.2.2 Derived SGAs From Known Energy Spectra

We want to introduce a method developed by Kumei [62] as stated in chapter 10.4 , p.311, of Wulfman's book [54]. This method was developed to find symmetry generators of physical systems in case that the Hamiltonian in question is a function of operators whose energy eigenspectrum is known. Later we will apply it to our toy model of the square root Hamiltonian. For simplicity we set all prefactors equal to one and neglected the ground energy constant which will not influence our qualitative results. The number operator $\hat{n}$ commutes with $\hat{H}$, that is $\left[\hat{n}, \hat{H}\right] = 0$ and the ϕ_n form a basis for the number operator with eigenvalues $n \in \mathbb{N}$,

$$\hat{n}\phi_n = n\phi_n. \tag{684}$$

Furthermore the Hamiltonian operator $\hat{H}$ is a function $\lambda(\hat{n})$ with energy eigenvalues $E(n) := \lambda(n)$, in signs

$$\hat{H}\phi_n = \lambda(\hat{n})\phi_n = E(n)\phi_n. \tag{685}$$

Since the ϕ_n are supposed to form a basis of the Hilbert space, we can express a general state ψ satisfying the Schrödinger equation as $\psi = \sum_n c_n\phi_n(q)\exp(-iE(n)t)$ with constant coefficients $c_n \in \mathbb{R}$. For a general solution ψ and the eigenstates ϕ_n we have the Schrödinger equations

$$i\frac{\partial}{\partial t}\psi = \hat{H}\psi \quad \text{and} \quad \hat{H}\phi_n = E(n)\phi_n. \tag{686}$$

Our aim is to find a transformation that converts $\exp(iE(n)t)$ into $\exp(int)$. We define

$$\alpha := \ln\left(\frac{\hat{n}}{\lambda(\hat{n})}\right) \tag{687}$$

and the displacement operator

$$\hat{D} := \exp\left(\alpha t\frac{\partial}{\partial t}\right). \tag{688}$$

According to these definitions we can transform the time coordinate t to obtain

$$t' := \hat{D}t = e^{\alpha}t \quad \text{and} \quad \frac{\partial}{\partial t'} = \hat{D}\frac{\partial}{\partial t} = e^{-\alpha}\frac{\partial}{\partial t}. \tag{689}$$

The relations can be shown by expanding $\hat{D}$ in a power series. To transform the Schrödinger equation in eq. (686) we apply the operator $\hat{D}$ to it which yields

$$\hat{D}\left(\hat{H} - i\frac{\partial}{\partial t}\right)\hat{D^{-1}}\hat{D}\sum_n c_n\phi_n(q)\exp(-iE(n)t) = 0. \tag{690}$$

We apply the operator $\hat{D}$ to the single terms of the Schrödinger equation which gives

$$\hat{D}\hat{H}\hat{D}^{-1} = \hat{H}, \tag{691}$$

$$\hat{D}i\frac{\partial}{\partial t}\hat{D}^{-1} = e^{-\alpha}i\frac{\partial}{\partial t} = \frac{i\lambda(\hat{n})}{\hat{n}}\frac{\partial}{\partial t}, \tag{692}$$

$$\hat{D}\sum_n c_n\phi_n(q)\exp(-iE(n)t) = \sum_n c_n\phi_n(q)\exp(-int)\,. \tag{693}$$

Then the transformed Schrödinger equation becomes

$$\left(\hat{H} - \frac{i\lambda(\hat{n})}{\hat{n}}\frac{\partial}{\partial t}\right)\sum_n c_n\phi_n(q)\exp(-int) = 0. \tag{694}$$

With the help of a transformation of the time coordinate t to $t' = \frac{n}{E(t)}t$, we managed to transform the exponential $\exp(-iE(n)t)$ to $\exp(-int)$ which means that we gain an exponential of a linear function of n like in case of the harmonic oscillator as discussed in 14.3.

On the other hand we obtain from

$$i\frac{\partial}{\partial t}\phi_n(q)\exp(-int) = n\phi_n(n)\exp(-int) = \hat{n}\exp(-int) \tag{695}$$

the equality $\hat{n} = i\frac{\partial}{\partial t}$. So we are left with

$$\left(\hat{H} - \lambda(\hat{n})\right)\sum_n c_n\phi_n(q)\exp(-int) = 0 \tag{696}$$

or

$$\left(\hat{H} - \lambda(i\frac{\partial}{\partial t})\right)\sum_n c_n\phi_n(q)\exp(-int) = 0. \tag{697}$$

To find symmetry generators $\hat{Q}$, that is the members of the SGA, we seek following Kumei [62] and in agreement with the definitions for the SGAs given in section 20.1 for operators $\hat{Q}$ that fulfill

$$\left(\hat{H} - i\frac{\partial}{\partial t}\right)\hat{Q}\psi = 0. \tag{698}$$

We apply the operator $\hat{D}$ to the equation

$$\hat{D}\left(\hat{H} - i\frac{\partial}{\partial t}\right)\hat{D}^{-1}\hat{D}\hat{Q}\hat{D}^{-1}\hat{D}\psi = 0 \tag{699}$$

and define $\hat{A} := \hat{D}\left(\hat{H} - i\frac{\partial}{\partial t}\right)\hat{D}^{-1} = \left(\hat{H} - \lambda(i\frac{\partial}{\partial t})\right)$, compare eq. (697). However, there is no further general guidance in [54] how to find the symmetry generators $\hat{Q}$ or $\hat{D}^{-1}\hat{D}\hat{Q}$. In [54] the method was applied to determine the SGA of rigid rotators.

Square Root Hamiltonian:
Now we consider as a toy model the square root Hamiltonian

$$\hat{H} = \sqrt{\hat{n}} \quad \text{and} \quad \sqrt{\hat{n}}\phi_n = \sqrt{n}\phi_n = \lambda(\hat{n})\phi_n = E(n)\phi_n. \tag{700}$$

In case of the square root Hamiltonian even the transformation $\hat{A} := \hat{D}\left(\hat{H} - i\frac{\partial}{\partial t}\right)\hat{D}^{-1}$ cannot be accomplished because in this setting we use that $\hat{n} = i\frac{\partial}{\partial t}$ derived from the eigenvalue equation to replace the number operator $\hat{n}$ in the expression for $\hat{A}$. However, we have

$$\hat{A} = \hat{D}\left(\sqrt{\hat{n}} - i\frac{\partial}{\partial t}\right)\hat{D}^{-1} = \left(\sqrt{\hat{n}} - \frac{i}{\sqrt{\hat{n}}}\frac{\partial}{\partial t}\right) = \left(\sqrt{i\frac{\partial}{\partial t}} - \frac{i}{\sqrt{i\frac{\partial}{\partial t}}}\frac{\partial}{\partial t}\right). \tag{701}$$

We obtain a fractional power of an operator. In momentum representation this becomes a fractional power of the momentum operator associated with the temporal coordinate which is a case considered in [63]. This brings us to the question whether we can find a time-rescaling that makes it possible to transform the system under consideration in such a way that the square root is going to vanish. The answer is to the affirmative and the searched transformation can be found with the help of the so-called dual Euler rescaling as will be discussed in section 22.1. In the context of semiclassical states we will also see there that it is helpful to go over to an extended phase space to find an effective Hamiltonian which does not include a fractional power of $\hat{n}$ anymore after the application of a dual Euler rescaling. By the construction of an effective Hamiltonian in section 22.1 we also connect to our idea from section 15.

21 Stability of Semiclassical States

In this section we start with a discussion about the meaning of stability and how it is achieved at least approximately in a practical approach. Next we display an abstract approach of what coherence breaking means and how it can be handled on an abstract level.

21.1 Stability Definitions

First we will summarize the variety of definitions for stability corresponding to different construction methods for semiclassical (coherent) states we encountered. For simplicity here we only consider time-independent Hamiltonian operators with a discrete spectrum.

21.1.1 Time-independent Harmonic Oscillator

Recall that the time-dependent coherent states for the harmonic oscillator $|\alpha, t\rangle$ can be obtained from the time-independent coherent states $|\alpha\rangle$ in eq. (529) by application of the unitary time-evolution operator $\hat{U}(t)$ associated with the time-dependent Schrödinger equation to $|\alpha\rangle$ which yields

$$|\alpha, t\rangle = \hat{U}(t)|\alpha\rangle = e^{-\frac{i}{\hbar}\hat{H}_{\mathrm{ho}}t}|\alpha\rangle = e^{-i\frac{\omega_0 t}{2}}|\alpha(t)\rangle, \tag{702}$$

where $\alpha(t) = \alpha\, e^{-i\omega_0 t}$. We calculate the expectation values of the position and momentum operators in the time-evolved coherent states $|\alpha, t\rangle$ leading to

$$\begin{aligned}\langle\alpha, t|\hat{q}|\alpha, t\rangle &= \langle\alpha(t)|\hat{q}|\alpha(t)\rangle = \sqrt{\frac{2\hbar}{m\omega_0}}\Re(\alpha(t)) = \sqrt{\frac{2\hbar}{m\omega_0}}|\alpha|\cos(\omega_0 t + \delta) \\ \langle\alpha, t|\hat{p}|\alpha, t\rangle &= \langle\alpha(t)|\hat{p}|\alpha(t)\rangle = \sqrt{2m\hbar\omega_0}\Im(\alpha(t)) = -\sqrt{2m\hbar\omega_0}|\alpha|\sin(\omega_0 t + \delta)\end{aligned} \tag{703}$$

with $\alpha = |\alpha|e^{-i\delta}$, $\delta \in \mathbb{R}$ which reassembles the expectation values for $\hat{q}$ and $\hat{p}$ in the coherent states $|\alpha\rangle$ for $t = 0$. This means that the expectation values of the position $\hat{q}$ and momentum operator $\hat{p}$ in the states $|\alpha\rangle$ or $|\alpha, t\rangle$, which correspond to the centre of the wave package, follow the classical trajectories $q(t)$ and $p(t)$ for all times t. Furthermore with

$$\langle\alpha|\hat{n}|\alpha\rangle = \langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle = \alpha^*\alpha\langle\alpha|\alpha\rangle = |\alpha|^2 \tag{704}$$

we can calculate

$$\langle\alpha|\hat{H}_{\mathrm{ho}}|\alpha\rangle = \langle\alpha, t|\hat{H}_{\mathrm{ho}}|\alpha, t\rangle = \hbar\omega_0\left(|\alpha|^2 + \frac{1}{2}\right). \tag{705}$$

This means that the expectation value of $\hat{H}_{\mathrm{ho}}$ in the coherent states $|\alpha, t\rangle$ reproduces the classical value in case we express α in terms of q and p. Consequently, $|\alpha, t\rangle$ are semiclassical and stable states for $\hat{q}$, $\hat{p}$ and $\hat{H}_{\mathrm{ho}}$ for all times $t \in \mathbb{R}^+$.

21.1.2 Phase States for $\mathfrak{A}_\kappa$

According to [40, 41] we discussed the phase states in section 16 in eq. (577) and stated some of their properties, especially their temporal stability in the sense of eq. (580), namely $e^{-iF(\hat{n})t}|\theta,\varphi\rangle = |\theta,\varphi+t\rangle$. Recall that the operator valued function $F(\hat{n})$ is equal to the Hamilton operator $\hat{H}$, i.e. $F(\hat{n}) = \hat{H}$ and n is the eigenvalue of the usual number operator $\hat{n}$ in the number operator eigenstates $|n\rangle$.

To investigate their stability behaviour we calculate

$$\langle\theta,\varphi+t|\hat{q}|\theta,\varphi+t\rangle = \sqrt{\frac{2\hbar}{m\omega_0}}\sum_{n=1}^{\infty}\sqrt{F(n)}\,\cos(\theta), \tag{706}$$
$$\langle\theta,\varphi+t|\hat{p}|\theta,\varphi+t\rangle = \sqrt{2m\omega_0\hbar}\sum_{n=1}^{\infty}\sqrt{F(n)}\,\sin(\theta)$$

for $\hat{q}$ and $\hat{p}$ as defined in section 16 and

$$\langle\theta,\varphi+t|F(\hat{n})|\theta,\varphi+t\rangle = \sum_{n=1}^{\infty}F(n) \tag{707}$$

which leads to the same diverging series's as discussed in section 16. So these states are no suitable semiclassical states in the sense that they should reproduce the classical value which is here $F(n)$, however they are stable in the sense that they lead to the same expectation value for all times t.

21.1.3 Klauder Coherent States

In section 17 we reviewed the construction of Klauder coherent states introduced in [33, 42] and displayed in the definition in eq. (602). Klauder et al. demand stability as a defining property for their coherent states and temporal stability is defined in the sense that for a coherent state with a classical label ℓ we have

$$e^{-i\hat{H}t}|\ell\rangle = |\ell(t)\rangle, \tag{708}$$

where $\hbar = 1$.
Under time evolution the states $|J,\gamma\rangle$ evolve as $e^{-i\hat{H}t}|J,\gamma\rangle = |J,\gamma+\omega t\rangle$ and are therefore stable according to his definition of stability. They satisfy the action identity for all times t, i.e.

$$\langle J,\gamma+\omega t|\hat{H}|J,\gamma+\omega t\rangle = \omega J \tag{709}$$

which comes from a comparison of the classical and "quantum" mechanical action integral. In this sense the expectation value of $\hat{H}$ in the Klauder coherent states reproduces by definition the classical value for all times $t \in \mathbb{R}^+$.

21.1.4 Complexifier Coherent States

In the definition of stability as displayed in [31] and section 18, the coherent state $|\phi_0\rangle := |\phi_{z(t_0)}\rangle$, with fixed $t_0 \in \mathbb{R}^+$ and $\hbar = 1$, will be a stable coherent state, if the equality

$$e^{-i\hat{H}(t-t_0)}|\phi_0\rangle = e^{i\beta(t)}|\phi_{z(t)}\rangle \tag{710}$$

holds for all $t \in \mathbb{R}^+$ and $z(t)$ follows the classical motion of $z(t_0)$ on the phase space which guarantees that this is still a coherent state, where $\exp(i\beta(t))$ is a phase factor with a real valued function $\beta(t)$.

21.2 Meaning of Stability

In section 21.1 we mentioned different definitions for the stability of states we have found in the literature [31, 33, 37, 40, 42]. Were the one in eq. (710) seems to be the most general one. These definitions of stability are all demands on the behaviour of the states under evolution with respect to a parameter t which in physics is usually the time. We see that the expectation values of certain operators in the defined states reproduce the classical values **for all times** t. Often this property is also taken as the defining property for stability: one says that a ***semiclassical state is stable*** if the expectation value of a certain operator in this state reproduces the classical value (up to small corrections) for all values of the parameter t. There might be small corrections in the sense of and according to the definition of a semiclassical state as explained in section 14.1.

A priory it is not clear that $e^{-i\hat{H}(t-t_0)}|\phi_0\rangle$ with $\hbar = 1$ gives again rise to a coherent or at least approximately coherent state at all. In the best case one can split the resulting time-evolved state in a coherent and comparatively small non-coherent part but neither is it clear that the state can be split into different parts nor that the non-coherent part is small. In the algebraic construction a coherent state is obtained by application of the exponential of linear combinations of representations of algebra generators $\hat{G}_i$ to a cyclic vector Ω (stays an element of the Hilbert space if one acts with a group element on it) which usually generates the elements of a group. The θ_i are constants $\in \mathbb{C}$ or complex valued functions which might label the classical phase space with $i \in \mathcal{I}$, where $\mathcal{I}$ is an arbitrary index set. Then the coherent state is given by

$$|\phi_0\rangle = e^{\sum_i \theta_i \hat{G}_i}|\Omega\rangle. \tag{711}$$

Now we can look at the time evolution of these states and check whether it is carried over to the "label" ϕ and so move it to the algebra to end up in a similar case as for the stability condition in eq. (710). Therefore, we consider

$$\begin{aligned} e^{-i\hat{H}t}|\phi_0\rangle &= e^{-i\hat{H}t}e^{\sum_i \theta_i \hat{G}_i}|\Omega\rangle \\ &= e^{-i\hat{H}t}e^{\sum_i \theta_i \hat{G}_i}e^{+i\hat{H}t}e^{-i\hat{H}t}|\Omega\rangle, \end{aligned} \tag{712}$$

where we set $t_0 = 0$ for simplicity and used the unitarity of the time-evolution operator $e^{+i\hat{H}t}e^{-i\hat{H}t} = \hat{\mathbb{1}}$. We can try to use the ***Baker-Campell-Hausdorff formula*** [159, 160, 161, 162] which states that

$$\hat{g}(t) = e^{-i\hat{H}t}\hat{g}e^{+i\hat{H}t} = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!}\left[\hat{H}, \hat{g}\right]_{(n)} \tag{713}$$

with $\left[\hat{H}, \hat{g}\right]_{(0)} = \hat{g}$ and $\left[\hat{H}, \hat{g}\right]_{(n)} = \left[\hat{H}, \left[\hat{H}, \hat{g}\right]_{(n-1)}\right]$ to write down an expression for the evolved state. In case that we set $\hat{g} = e^{\sum_i \theta_i \hat{G}_i}$ and apply the Baker-Campell-Hausdorff formula displayed in eq. (713) together with the operator (matrix) exponential we obtain

$$\begin{aligned}\hat{g}(t) &= \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \left[\hat{H}, \hat{g}\right]_{(n)} = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \left[\hat{H}, e^{\sum_i \theta_i \hat{G}_i}\right]_{(n)} \qquad (714)\\ &= \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \left[\hat{H}, \sum_{\ell=0}^{\infty} \frac{\left(\sum_i \theta_i \hat{G}_i\right)^\ell}{\ell!}\right]_{(n)}\\ &= \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \left[\hat{H}, \left(\sum_i \theta_i \hat{G}_i\right)^\ell\right]_{(n)} .\end{aligned}$$

To calculate this expression we need to know the commutators $\left[\hat{H}, \hat{G}_i\right]$. Alternatively, we have

$$\begin{aligned}\hat{g}(t) &= e^{-i\hat{H}t} e^{\sum_i \theta_i \hat{G}_i} e^{+i\hat{H}t} \qquad (715)\\ &= e^{-i\hat{H}t} \sum_{\ell=0}^{\infty} \frac{\left(\sum_i \theta_i \hat{G}_i\right)^\ell}{\ell!} e^{+i\hat{H}t} = \sum_{\ell=0}^{\infty} \frac{1}{\ell!} e^{-i\hat{H}t} \left(\sum_i \theta_i \hat{G}_i\right)^\ell e^{+i\hat{H}t}\\ &= \sum_{\ell=0}^{\infty} \frac{1}{\ell!} e^{-i\hat{H}t} \underbrace{\left(\sum_i \theta_i \hat{G}_i\right) \cdot \ldots \cdot \left(\sum_i \theta_i \hat{G}_i\right)}_{\ell \text{ times}} e^{+i\hat{H}t}\\ &= \sum_{\ell=0}^{\infty} \frac{1}{\ell!} e^{-i\hat{H}t} \left(\sum_i \theta_i \hat{G}_i\right) \cdot \mathbb{1} \ldots \mathbb{1} \cdot \left(\sum_i \theta_i \hat{G}_i\right) e^{+i\hat{H}t}\\ &= \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \left(e^{-i\hat{H}t} \sum_i \theta_i \hat{G}_i e^{+i\hat{H}t}\right) \cdot \ldots \cdot \left(e^{-i\hat{H}t} \sum_i \theta_i \hat{G}_i e^{+i\hat{H}t}\right)\\ &= \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \left(e^{-i\hat{H}t} \sum_i \theta_i \hat{G}_i e^{+i\hat{H}t}\right)^\ell = e^{\left(e^{-i\hat{H}t} \sum_i \theta_i \hat{G}_i e^{+i\hat{H}t}\right)} =: e^{\sum_i \theta_i \hat{G}_i(t)}\end{aligned}$$

and for the power we could again use eq. (713) to rewrite

$$\sum_i \theta_i \hat{G}_i(t) = e^{-i\hat{H}t} \sum_i \theta_i \hat{G}_i e^{+i\hat{H}t} = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \left[\hat{H}, \sum_i \theta_i \hat{G}_i\right]_{(n)} . \qquad (716)$$

Both options show us that it is very important to calculate the commutators of the Hamiltonian operator $\hat{H}$ with the algebra elements and consider them as new algebra elements to get the dynamical input. Here we refer to Dothan who showed in [53] that if one considers only the evolved kinematical position and momentum operators as displayed in eq. (648) in section 20.1.1, then the algebra will always be isomorphic to the Weyl-Heisenberg algebra. However, this is only the kinematical input and not the dynamical one which comes in by adding the commutators of $[\hat{H}, (\sum_i \theta_i \hat{G}_i)^\ell]_{(n)}$ to the algebra.

Next we compare the stability criterion with the evolved coherent state from the algebraic construction that is

$$e^{-i\hat{H}t}|\phi_0\rangle = e^{-i\hat{H}t} e^{\sum_i \theta_i \hat{G}_i}|\Omega\rangle = e^{\sum_i \theta_i \hat{G}_i(t)} e^{-i\hat{H}t}|\Omega\rangle \overset{!}{=} e^{i\beta(t)}|\phi_{z(t)}\rangle, \qquad (717)$$

where we further assume that $|\phi_0\rangle = |\phi_{z(t_0)}\rangle$ for a fixed time $t_0 \in \mathbb{R}$.

Suppose that we have an instable system, that is

$$e^{\sum_i \theta_i \hat{G}_i(t)} e^{-i\hat{H}t}|\Omega\rangle \neq e^{i\beta(t)}|\phi_{z(t)}\rangle. \tag{718}$$

Can we stabelize the states somehow? Or define approximately stable coherent states? Naively one could think about multiplying the cyclic vector (vacuum state) Ω by an exponential to the power of a function which exactly annihilates the terms coming from the application of $e^{\sum_i \theta_i \hat{G}_i(t)} e^{-i\hat{H}t}$ to Ω causing the instability or more generally by something like the inverse function of the function causing the instability. Here again the question arises what are the parts of $\hat{G}_i$ which cause the instability and can we split $\hat{H}$ into parts that leave ϕ_0 stable or not. Furthermore would this so modified state still describe the correct dynamics of the system?

Let our starting point be a set of generators $\hat{G}_i$ $i = 0, 1, 2...$ and we set $\hat{G}_0 := \hat{H}$ and we know the commutators $[\hat{G}_i, \hat{G}_j]$ for $i, j > 0$. We saw that especially to consider the dynamics of the given physical problem we need to calculate the commutators $[\hat{H}, \hat{G}_k]$ for $k \in \mathbb{N}_0$.

We collect some possible cases:

1. Special case $[\hat{H}, \hat{G}_k] = 0$ and $\hat{G}_k$ is not explicitly time-dependent, that is $\hat{G}_k$ is a constant of motion.
2. $[\hat{G}_i, \hat{G}_k] = c^j_{ik}\hat{G}_j$ with structure constants c^j_{ik}, i.e. Lie algebra.
3. $[\hat{G}_i, \hat{G}_k] = F(\hat{G}_j)$ a function of generators $F(\hat{G}_j)$.
4. $[\hat{G}_i, \hat{G}_k] = f^j_{ik}$(phase space variables)$\hat{G}_j$ with structure functions f^j_{ik}(phase space variables), i.e. Lie algebroid.

Another important aspect which needs to be taken into account is the finiteness or infiniteness of the number of generators, i.e. is the algebra closed or not. Let us examine the commutator $[\hat{G}_i, \hat{G}_k] = F(\hat{G}_j)$, then $F(\hat{G}_j)$ might be an element of the algebra we already know, i.e. $F(\hat{G}_j) = \hat{G}_i$ or it might be a new element which we can add to the algebra and calculate all commutators with all the other elements which might generate more and more elements. This process can stop at some point or go on infinitely often. Consequently, the algebra is not closed and infinitely large. Notice that for finitely many degrees of freedom as discussed in [53] or section 20 it should be possible to find a representation of the generators in which the algebra is closed.

Now we evaluate our cases from above:

1. In many cases we know the eigenvalue equation for the non-time dependent Hamiltonian operator $\hat{H}|\Omega\rangle = \kappa(.)|\Omega\rangle$ for $\kappa(.)$ being a real valued function maybe depending on the eigenvalues of some other generators of the algebra. The stability condition becomes

$$e^{\sum_i \theta_i \hat{G}_i(t)} e^{-i\hat{H}t}|\Omega\rangle = e^{-i\kappa(.)t} e^{\sum_i \theta_i \hat{G}_i(t)}|\Omega\rangle. \tag{719}$$

We define $\beta(t) := -\kappa(.)t + \delta(t)$ with a real valued function $\delta(t)$ and identify

$$e^{\sum_i \theta_i \hat{G}_i(t)}|\Omega\rangle = e^{i\delta(t)}|\phi_{z(t)}\rangle. \tag{720}$$

Clearly if, $[\hat{H}, \hat{G}_k] = 0$ and $\hat{G}_k$ is not explicitly time-dependent, then we are left with

$$\begin{aligned} e^{\sum_i \theta_i \hat{G}_i(t)} e^{-i\hat{H}t}|\Omega\rangle &= e^{\sum_i \theta_i \hat{G}_i} e^{-i\hat{H}t}|\Omega\rangle \\ &= e^{-i\kappa(.)t} e^{\sum_i \theta_i \hat{G}_i}|\Omega\rangle \\ &= e^{-i\kappa(.)t}|\phi_0\rangle \end{aligned} \tag{721}$$

which is by definition a coherent state.

2. In case of a Lie algebra $[\hat{G}_i, \hat{G}_k] = c_{ik}^j \hat{G}_j = \sum_j c_{ikj}\hat{G}_j$ and $\hat{G}_0 := \hat{H}$, we can use the Baker-Campell-Hausdorff formula in eq. (713) to calculate the exponent

$$\left(e^{-i\hat{H}t}\sum_i \theta_i \hat{G}_i e^{+i\hat{H}t}\right) = \sum_{n=0}^{\infty}\frac{(-it)^n}{n!}\left[\hat{H}, \sum_i \theta_i \hat{G}_i\right]_{(n)} . \tag{722}$$

We have

$$\begin{aligned}
\left[\hat{H}, \sum_i \theta_i \hat{G}_i\right]_{(0)} &= \sum_i \theta_i \hat{G}_i \\
\left[\hat{H}, \sum_i \theta_i \hat{G}_i\right]_{(1)} &= \sum_i \theta_i \left[\hat{H}, \hat{G}_i\right] = \sum_i\sum_k \theta_i c_{0ik}\hat{G}_k \\
\left[\hat{H}, \sum_i \theta_i \hat{G}_i\right]_{(2)} &= \left[\hat{H}, \left[\hat{H}, \sum_i \theta_i \hat{G}_i\right]\right] \\
&= \sum_{i,k}\theta_\ell c_{0ik}\left[\hat{G}_0, \hat{G}_k\right] = \sum_{i,k}\sum_\ell \theta_i c_{0ik}c_{0k\ell}\hat{G}_\ell .
\end{aligned} \tag{723}$$

What we see is that we always obtain a linear combination of generators in case of a Lie algebra. Keep in mind that in general the sums possibly do not converge. Assume that after N iteration steps all commutators vanish, i.e. $\left[\hat{H}, \sum_i \theta_i \hat{G}_i\right]_{(n)} = 0$ for $n > N \in \mathbb{N}$. We obtain a polynomial in the generators in the time-parameter t of degree N which is related to the discussion in [53] but without an explicit construction be given there

$$\begin{aligned}
\left(e^{-i\hat{H}t}\sum_i \theta_i \hat{G}_i e^{+i\hat{H}t}\right) &= \sum_{n=0}^{N}\frac{(-it)^n}{n!}\left[\hat{H}, \sum_i \theta_i \hat{G}_i\right]_{(n)} \\
&= \sum_i \theta_i \hat{G}_i + \sum_{n=1}^{N}\frac{(-it)^n}{n!}\sum_i\sum_{k_1,\ldots k_n}\theta_i c_{0ik_1}\prod_{j=1}^{n-1} c_{0k_jk_{j+1}}\hat{G}_{k_n}
\end{aligned} \tag{724}$$

with the action

$$\begin{aligned}
e^{\sum_i \theta_i \hat{G}_i(t)}e^{-i\hat{H}t}|\Omega\rangle &= e^{\sum_{n=0}^N \frac{(-it)^n}{n!}\left[\hat{H},\sum_i \theta_i\hat{G}_i\right]_{(n)}}e^{-i\hat{H}t}|\Omega\rangle \\
&= e^{-i\kappa(.)t}e^{\sum_{n=0}^N \frac{(-it)^n}{n!}\left[\hat{H},\sum_i \theta_i\hat{G}_i\right]_{(n)}}|\Omega\rangle \\
&= e^{-i\kappa(.)t}e^{\sum_i \theta_i\hat{G}_i + \sum_{n=1}^N \frac{(-it)^n}{n!}\left[\hat{H},\sum_i \theta_i\hat{G}_i\right]_{(n)}}|\Omega\rangle \\
&= e^{-i\kappa(.)t}e^{\sum_i \theta_i\hat{G}_i + \sum_{n=1}^N \frac{(-it)^n}{n!}\sum_i\sum_{k_1,\ldots k_n}\theta_i c_{0ik_1}\prod_{j=1}^{n-1}c_{0k_jk_{j+1}}\hat{G}_{k_n}}|\Omega\rangle .
\end{aligned} \tag{725}$$

As we have seen above the “zero order” part $e^{-i\kappa(.)t}e^{\sum_i \theta_i\hat{G}_i}$ applied to $|\Omega\rangle$ is stable. The rest of the sum is an exponentiated polynomial in $-it$ times a complex linear combination of the Generators. One can of course replace t by a small time interval Δt and recalculate the states, then they would approximately be stable.

Cases 3. and 4. might be handeled in a similar way depending on the exact form of the functional dependence of $F(\hat{G}_j)$ or the phase space function f_{ik}^j(phase space variables).

21.3 Expectation Values

Before we go on with the stability discussion, we want to discuss the calculation of expectation values of the generators $\hat{G}_i$ in the group coherent states given by

$$\langle\phi_0|\hat{G}_k|\phi_0\rangle = \langle\Omega|e^{\sum_i \theta_i^* \hat{G}_i^\dagger}\hat{G}_k e^{\sum_i \theta_i \hat{G}_i}|\Omega\rangle. \tag{726}$$

According to the construction principle for group coherent states, we assume that $e^{\sum_i \theta_i \hat{G}_i}$ is a unitary operator. So we want that

$$\begin{aligned} &e^{\sum_i \theta_i^* \hat{G}_i^\dagger} e^{\sum_i \theta_i \hat{G}_i} = \mathbb{1} \\ \Rightarrow &\sum_i \theta_i^* \hat{G}_i^\dagger = \left(\sum_i \theta_i \hat{G}_i\right) = -\sum_i \theta_i \hat{G}_i. \end{aligned} \tag{727}$$

With this the expectation value becomes

$$\begin{aligned} \langle\phi_0|\hat{G}_k|\phi_0\rangle &= \langle\Omega|e^{-\sum_i \theta_i \hat{G}_i}\hat{G}_k e^{\sum_i \theta_i \hat{G}_i}|\Omega\rangle = \langle\Omega|e^{-\sum_i \theta_i \hat{G}_i}\hat{G}_k e^{-\left(-\sum_i \theta_i \hat{G}_i\right)}|\Omega\rangle \\ &= \langle\Omega|\sum_{m=0}^{\infty}\frac{1}{m!}\left[-\sum_i \theta_i \hat{G}_i, \hat{G}_k\right]_{(m)}|\Omega\rangle. \end{aligned} \tag{728}$$

Again we use the Baker-Campell-Hausdorff formula from eq. (713) which yields

$$\begin{aligned} \left[\sum_i \theta_i \hat{G}_i, \hat{G}_k\right]_{(0)} &= \hat{G}_k, \\ \left[\sum_i \theta_i \hat{G}_i, \hat{G}_k\right]_{(1)} &= \sum_i \sum_\ell \theta_i c_{ik\ell}\hat{G}_\ell, \\ \left[\sum_i \theta_i \hat{G}_i, \hat{G}_k\right]_{(2)} &= \left[\sum_i \theta_i \hat{G}_i, \left[\sum_i \theta_i \hat{G}_i, \hat{G}_k\right]\right] = \sum_{i_1,i_2}\theta_{i_1}\theta_{i_2}\sum_\ell c_{i_1 k \ell_1} c_{i_2 \ell_1 \ell_2}\hat{G}_{\ell_2} \end{aligned} \tag{729}$$

... etc. from this we deduce that

$$\langle\phi_0|\hat{G}_k|\phi_0\rangle = \langle\Omega|\sum_{m=0}^{\infty}\frac{(-1)^m}{m!}\sum_{i_1,\ldots,i_m}\sum_{\ell_0,\ldots,\ell_m}\prod_{p=1}^{m}\theta_{i_p}\prod_{x=1}^{m}c_{i_x \ell_{x-1}\ell_x}\hat{G}_{\ell_m}|\Omega\rangle, \tag{730}$$

where we set $\ell_0 := k$. We define

$$M_{\ell_{x-1}\ell_x} := \theta_{i_x} c_{i_x \ell_{x-1}\ell_x} \tag{731}$$

using this the expectation value becomes

$$\begin{aligned} \langle\phi_0|\hat{G}_k|\phi_0\rangle &= \langle\Omega|\sum_{m=0}^{\infty}\frac{(-1)^m}{m!}\sum_{\ell_0,\ldots,\ell_m} M_{\ell_0\ell_1}\cdot\ldots\cdot M_{\ell_{m-1}\ell_m}\hat{G}_{\ell_m}|\Omega\rangle \\ &= \langle\Omega|\exp(-M_{k\ell})\hat{G}_\ell|\Omega\rangle = \left(e^{-M}\right)^{k\ell}\langle\Omega|\hat{G}_\ell|\Omega\rangle, \end{aligned} \tag{732}$$

since the matrix M contains only complex numbers, maybe complex valued functions θ_i and structure constants we can pull the matrix exponential out of the expectation value.

Instead of trying to find a stable coherent state for a given algebra or calculable algebra, one can also change the point of view and ask: given a certain stable coherent or semiclassical state for a physical system, how can we change the physical system described by the Hamiltonian operator such that the state is still a stable coherent or semiclassical state for the changed system?

21.4 Known Stability Results

Several authors, beginning with Glauber [56], and followed for example by [57, 58, 59, 60] discussed what form the Hamiltonian is allowed to have or more specific what elements it is allowed to contain to leave a given coherent state coherent, i.e. stable. Earlier works mainly concern generalizations of the harmonic oscillator with the result that the most general Hamiltonian operator that preserves the coherent states of the N-dimensional harmonic oscillator $|\alpha\rangle = |\alpha_1, \ldots, \alpha_N\rangle$ is

$$\hat{H}(t) = \sum_{\ell,k=1}^{N} \omega_{\ell k}(t) \hat{a}_\ell^\dagger \hat{a}_k + \sum_{k=1}^{N} (F_k(t)\hat{a}_k + F_k^*(t)\hat{a}_k^\dagger) + \xi(t) \tag{733}$$

for a complex valued function $F(t)$ and real valued functions $\omega_{\ell k}(t)$ and $\xi(t)$ which all might depend on a time parameter $t \in \mathbb{R}^+$. Also if $\hat{H} = G(\hat{a})$ is a function of $\hat{a}$ it will preserve $|\alpha\rangle$, where we left out possible multi-indices for more than one dimension. In the context of the complexifier construction for coherent states Zipfel gave in [31] a more general proof that Hamiltonian operators which only depend on annihilation operators, where the concept of annihilation operator in the context of the construction of the complexifier coherent states is used, leave the complexifier coherent states stable, see section 18. They tried to circumvent the problem of instability in [31] by changing to new phase space functions on the classical level using the Hamilton-Jacobi equations, i.e. canonical transformations which then might become only annihilation operators in the generalized sense explained in their article. However, this transformation in general works only locally.

In [61] they show that the most general Hamiltonian operator $\hat{H}$ that preserves a coherent state $|\phi_0\rangle \in M$, where M is a homogeneous space, is an element of the extension of the Lie algebra $\mathfrak{g}$ of G by the algebra $\mathfrak{a} = \mathfrak{s}/\mathfrak{g}$. Here $\mathfrak{s}$ is the algebra associated with the group of automorphisms of M, $\mathcal{G} = Aut(M)$, that is $\hat{H} \in \mathfrak{s}$. One can realize $\mathcal{G} = Aut(M)$ by the adjoint representation $\mathrm{Ad}(\mathcal{G})$. According to [61] the following properties of Lie groups give us the guidelines how to find $\mathfrak{s}$, for the definitions of the group properties see section 19:

- If G is ***semisimple*** $\longrightarrow$ $\mathfrak{s}$ coincides with $\mathfrak{g}$ up to identity automorphisms, since $\mathcal{G} = G \times D$, where D is a discrete group and $\mathrm{Ad}(\mathcal{G}) \cong \mathcal{G} \Rightarrow \hat{H} \in \mathfrak{g} \Rightarrow G$ is the dynamical group.
- If G is ***solvable*** $\longrightarrow$ $\mathfrak{s} = \mathfrak{a} \oplus \mathfrak{g}$, where $\mathfrak{g}$ is a maximal solvable ideal and $\mathfrak{a}$ is a Lie algebra that preserves $|\Omega\rangle$ and $|\phi_t\rangle := U(t,t_0)|\phi_0\rangle = \mathrm{Ad}(s)U(gs)|\Omega\rangle$ (except a phase factor) for $g \in G$ and $s \in \mathcal{G}$ is a coherent state, if both G and h are invariant subgroups of $\mathcal{G}$.
- If G is ***compact*** $\rightarrow$ $|\Omega\rangle$ can be chosen to be the highest weight vector of the irreducible representation $U(g)$.

In order to preserve the coherence of the initial state the time-evolution operators are required to be in one-to-one correspondence with the elements of $\mathcal{G}$.

21.4.1 Breaking the Coherence

From the knowledge of the form of the most general Hamiltonian that preserves the coherence, the questions arises what happens in case one adds terms or more general a function to the Hamiltonian which breaks the coherence. For this purpose they consider in [61] the coherence breaking part to be a time-dependent function $W(t)$ of compact support and assumed that $W(t)$ is a small perturbation in comparison to the coherence preserving Hamiltonian H. We learned from [61] that the Hamiltonian preserves the coherence if it is an element of $\mathfrak{s}$, i.e. $H \in \mathfrak{s}$. As shown in [61] and displayed in appendix I the coherence breaking functions are elements of the algebra

$$\mathfrak{U} = \bigcup_{2 \leq p \leq k} \mathfrak{E}^{(p)}/\mathfrak{s}, \tag{734}$$

where k is a integer greater or equal to 2 and $\mathfrak{E}^{(p)}$ is the universal enveloping algebra of order p of the algebra $\mathfrak{g}$ corresponding to the Lie group G. In a visual way the universal enveloping algebra is the algebra build by all possible combinations and powers of the elements of the algebra $\mathfrak{g}$. Consequently, the algebra $\mathfrak{U}$ is the universal enveloping algebra without the elements belonging to $\mathfrak{s}$.

On an abstract level the proof in [61] and displayed in appendix I explains how to find coherent states for every system covered by the proof. However, the proof does not give a practical implementation of those states. The course of the proof gives a hint that one should watch out for variables which are functions of the original variables the system is described in, such that the algebra in these new variables is isomorphic to the algebra of the original system. This is in accordance with considerations about preserving simplectic structures when searching for new variables to describe a physical system. Hence, we are encouraged to look for canonical transformations.

In the two upcoming sections we will finally combine our gained knowledge about the construction of semiclassical or coherent states. The inverse Thiemann identity in section 15 and the Kumei method in section 20.2.2 brought us to the idea to search for a possibility to rescale the time coordinate such that includes the square root in some way such that we can define an effective Hamiltonian. Our considerations about phase states in section 16, the algebraic construction in section 19, the spectrum generating algebras 20 and especially what leaves a coherent states coherent in section 21 brought us to the point that even for the square root or more general fractional Hamiltonians we should be able to use the original or an isomorphic algebra, which in case of our toy model is just the Weyl-Heisenberg algebra, to construct semiclassical states.

22 Physical Coherent States for Constrained Systems

Large parts of this section are contained in the article [71]. There exists already preliminary work on the construction of coherent states for constrained systems in the literature, like for instance in [64, 163] where physical coherent states for constrained systems were constructed. In [163] the physical coherent states are deduced from the inclusion of constraints into the framework of quantum mechanical path integrals which results in projecting a state from the kinematical Hilbert space into a state in the physical Hilbert space. The article concludes with the application of this method to time reparametrization invariant systems, which for example occur in quantum gravity. The method in [64] starts from known kinematical harmonic oscillator coherent states and projects them with the help of group averaging to the physical Hilbert space. If it is assumed that the coherent states are peaked on the classical constraint surface, the results in [67] show that physical coherent states as well as their inner product can be obtained. For an application in cosmology to Bianchi I spacetimes, see [164]. The work in [64] considers constraints with an either linear or quadratic dependence on the elementary phase space variables only. In this section we want to follow closely the methods introduced in [64] but now apply them to constraints that involve fractional powers of the elementary phase space variables.

22.1 Euler Rescaling as a Canonical Transformations on the Extended Phase Space

Large parts of this section are contained in the article [71]. In order to deal with a constrained system with a fractional power of a Hamiltonian, for which not necessarily semiclassical perturbation theory explained in part IV can be applied, we work in the extended phase space. As discussed in [114] coherent states for a constrained system will in general have some restriction on their label in order to ensure that their labels are consistent with the constraints of the system. Here we want to combine this idea with the one of semiclassical perturbation theory and use a canonical transformation, the so-called dual Euler rescaling, to obtain, as in case of semiclassical perturbation theory, a substitution for our fractional power Hamiltonian in terms of integer powers that has the required properties as far as the semiclassical limit is considered. We will restrict our discussion to fractional powers of the harmonic oscillator Hamiltonian here. However, the strategy can be carried over to more complicated systems, if the constraint associated with temporal diffeomorphisms (for General Relativity this is the Hamiltonian constraint), can be written in deparametrized[2] form at the classical level and the set of coherent states that one wants to use for the computations have good semiclassical properties as far as integer powers of the Hamiltonian are considered. We will discuss this aspect in more detail in our conclusions in section 24. To explain how the Euler rescaling can be useful in this context, let us consider the following set up: we examine a Hamiltonian that is given by some fractional power of the harmonic oscillator in one dimension formulated on the phase space T^*Q with elementary variables (q,p). We denote the Hamiltonian as $H_{\rm ho}^{\mu}$ where μ is a rational number $\mu = \frac{v}{w}$ with $v, w \in \mathbb{N}$ and $H_{\rm ho}$ is the Hamiltonian of the harmonic oscillator that is given by $H_{\rm ho} = \frac{p^2}{2m} + \frac{m\omega_0^2 q^2}{2}$. In order to map this dynamical system into a constrained system with a deparametrized constraint we work in the extended phase space T^*M in which the temporal coordinate is also treated as a canonical variable with coordinates (t, p_t, q, p). The constraint of the system in the extended phase space has the form

$$C = k(p_t + H_{\rm ho}^{\mu}), \quad \{q,p\} = 1, \quad \{t, p_t\} = 1, \tag{735}$$

where k is some arbitrary real and non-zero number and all remaining Poisson brackets vanish. Let us briefly comment on the units of the involved quantities. From the constraint C we can read off that $[p_t] = [\text{energy}]^{\mu} = J^{\mu}$. Furthermore we have $[q] = [\text{length}] = m$, $[p] = [force \times time] = Ns$ and $[t] = J^{-\mu+1}s$. Here deparametrization means that the constraint can be written linearly in the temporal momentum and the remaining part of the constraint does not include t. In the extended phase space as shown for instance in [165], we can write down a set of first order Hamilton's equation with respect to an evolution parameter that we denote by s

$$\frac{dq(s)}{ds} = k\{q(s), H_{\rm ho}^{\mu}\}, \quad \frac{dp(s)}{ds} = k\{p, H_{\rm ho}^{\mu}\}, \quad \frac{dt}{ds} = \{t, C\} = k, \quad \frac{dp_t(s)}{ds} = \{p_t, C\} = 0. \tag{736}$$

Now what we are interested in a constrained system is the dynamics of the observables, which are phase space functions in the so-called reduced phase space. The reduced phase space can be obtained by a symplectic reduction with respect to C and can be coordinatized by the corresponding elementary observables associated with q, p. These observables are quantities that are required to commute with the constraint C. From now on let us consider the choice $k = 1$. In this case the the physical Hamiltonian, which generates the evolution of the observables, is then

[2] Deparametrization in this context means that the constraint can be written as $C = p_T + h$, where p_T denotes the momentum of the configuration variable playing the role of the clock of the system and h involves only the remaining phase space variables but not the one from the clock degrees of freedom.

given by the function $H^{\mu}_{\rm ho}$ evaluated at the observables of q and p. Let us denote the observables of q, p by O_q and O_p, then the classical Hamilton's equation in the reduced phase space read:

$$\frac{dO_q}{d\tau} = \{O_q(\tau), H^{\mu}_{\rm ho}(O_q, O_p)\}, \quad \frac{dO_p(\tau)}{d\tau} = \{O_p, H^{\mu}_{\rm ho}(O_q, O_p)\}, \tag{737}$$

where we denoted the evolution parameter in the reduced phase space by τ to match with our later notation at the end of section 22.3. We realize that for the choice $k = 1$ and under the identification $O_q \to q$, $O_p \to p$ and $\tau \to s$ the Hamilton's equations in eq. (736) and eq. (737) agree for this subset of variables. In this sense we can cast any classical Hamiltonian system with a given Hamiltonian H into a constrained system with constraint $C = p_t + H$ in the extended phase space that is written linearly in the temporal momentum. Looking at the equations of motion in eq. (736) with $k = 1$, we realize that the outer derivative of $H^{\mu}_{\rm ho}$ involved the first order equations for $\frac{dq}{ds} = \mu H^{\mu-1}_{\rm ho}\{q, H_{\rm ho}\}$ and likewise for $\frac{dp}{ds}$ can be absorbed into a redefinition of the temporal coordinate and with respect to the transformed time the Hamiltonian is just linear in the harmonic oscillator Hamiltonian $H_{\rm ho}$. In the extended phase space this can be formulated as a canonical transformation of the form

$$P_T = |p_t|^{\frac{1}{\mu}}\mathrm{sgn}(p_t), \quad T = \mathrm{sgn}(p_t)\frac{\mu t}{|p_t|^{\frac{1}{\mu}-1}}, \quad Q = q, \quad P = p. \tag{738}$$

The variables (T, P_t) have the units $[P_T] = J$ and $[T] = s$. This transformation often denoted as Euler rescaling was discussed in a more general context for instance in [165]. Note that in our case this is rather a kind of dual Euler rescaling, since here the new temporal momentum P_T is a function of p_t only, whereas the new temporal coordinate T is a function of t, p_t. In contrast to the Euler rescaling in [165] the new temporal variable T is a function of t only and P_T a function of t, p_t. Furthermore in [165] the transformation to t involves an integral. Assuming that $p_t \neq 0$, we can multiply the entire constraint C by $|p_t|^{\frac{1}{\mu}-1}\mathrm{sgn}(p_t)$ and obtain

$$\widetilde{C} = |p_t|^{\frac{1}{\mu}} + |p_t|^{\frac{1}{\mu}-1}\mathrm{sgn}(p_t)H^{\mu}_{\rm ho} \approx |p_t|^{\frac{1}{\mu}} - H_{\rm ho}H^{-\mu}_{\rm ho}\mathrm{sgn}(H_{\rm ho})H^{\mu}_{\rm ho} = |p_t|^{\frac{1}{\mu}} - H_{\rm ho}, \tag{739}$$

where we used the weak $\approx$ equivalence of quantities on the constraint surface $C = 0$ and that $\mathrm{sgn}(H_{\rm HO}) = 1$ since $H_{\rm HO} > 0$. In this sense the new constraint $\widetilde{C}$ implies $p_t = -H^{\mu}_{\rm ho}$ on the constraint surface which requires $p_t < 0$ and thus $-p_t = |p_t| \approx H^{\mu}_{\rm ho}$ leading to $|p_t|^{\frac{1}{\mu}} \approx H_{\rm ho}$. An important property of the above defined canonical transformation is that p_t, and thus also any function of it, is a constant of motion which on the reduced phase space can be identified with the energy of the physical system. As a consequence, when we use the rewritten and equivalent version of the constraint in eq. (739) in the next section to construct coherent states in constrained systems, we have to take this into account and consider that not $H_{\rm ho}$ is the energy of our original system that we start from but $H^{\mu}_{\rm ho}$ and thus $H_{\rm HO} = |p_t|^{\frac{1}{\mu}} = (E^{(s)})^{\frac{1}{\mu}}$, where $E^{(s)}$ denotes the energy of the system and can be determined once the phase space variables are given. To keep track of the original definition of the energy of the system before the dual Euler rescaling has been applied goes in the same direction as the idea of a kind of reference metric suggested by Klauder in [166] in order to be able to have a consistent interpretation of the dynamical operator even if a transformation of the phase space variables has been applied.

If we want to work with the constraint $\widetilde{C}$ in eq. (739), then it will look like that we have not gained much, since we just moved the fractional power from the Hamiltonian to the momentum p_t. However, as shown in [63] using Kummer functions fractional powers of the momentum operator can be well approximated by the standard harmonic oscillator coherent states and we will use those results here to obtain appropriate coherent states on the kinematical Hilbert space which approximate the quantum constraint well semiclassically.

Now given the constraint in the form we wanted, we can proceed in two directions. Either we consider Dirac quantization and solve the constraint in the quantum theory or we derive the reduced phase at the classical level and apply reduced phase space quantization. At this stage both are equally justified. In the context of coherent states this carries over to the situation that when applying Dirac quantization those coherent states are usually constructed on the kinematical Hilbert space. However, in order to actual compute relevant semiclassical expectation values one would like to use physical coherent states that encode some information about the constraints in the system. As mentioned at the beginning of this section a strategy to obtain physical coherent states from a given set of kinematical coherent states was presented in [64] and applied to a couple of examples there. We will summarize this strategy in the next section and apply it in section 22.3 to fractional Hamiltonians combined with the dual Euler rescaling just discussed, where this technique is still based on using the standard harmonic oscillator coherent states. At the end of the section 22.3 we will also show that in this case reduced phase space quantization and Dirac quantization will yield to the same set of physical coherent states.

22.2 Introduction to the Construction of Physical Constrained Coherent States

In [64] physical coherent states for constrained systems were constructed from given kinematical coherent states via group averaging. To be able to define kinematical coherent states, systems with D degrees of freedom with linear phase spaces $\Gamma = \mathbb{R}^{2D}$ were considered. For these phase spaces each phase space point γ can be described by a canonical coordinate basis (q_i, p_i) with $i = 1, 2, \dots, D$. The linear phase space Γ serves as the kinematical phase space which can be quantized in a standard fashion using Fock quantization leading to the kinematical Hilbert space $\mathcal{H}_{\text{kin}}$. In order to quantize the linear phase space Γ one defines the dimensionless holomorphic coordinates, similar to the case of the harmonic oscillator,

$$z_i := \frac{q_i}{\sqrt{2}\ell_i} + i\frac{\ell_i p_i}{\sqrt{2}\hbar}, \tag{740}$$

where we introduced the scale ℓ_i with dimension of length and there is no summation over i here. For a specific point α in Γ with coordinates (q_i^0, p_i^0) one sets

$$\alpha_i := \frac{q_i^0}{\sqrt{2}\ell_i} + i\frac{\ell_i p_i^0}{\sqrt{2}\hbar}. \tag{741}$$

When we go over to the quantum theory the z_i become the well known boson annihilation operators $\hat{a}_i$ with adjoint creation operators $\hat{a}_i^\dagger$ and they satisfy the commutation relations $\left[\hat{a}_i, \hat{a}_j^\dagger\right] = \hat{\mathbb{1}}\delta_{ij}$. The kinematical normalized coherent states are then given by

$$\begin{aligned} |\Psi_\alpha\rangle &= e^{\sum_{i=0}^{D}\left(\alpha_i\hat{a}_i^\dagger - \bar{\alpha_i}\hat{a}_i\right)}|0\rangle = \bigotimes_{i=1}^{D}\left[e^{-\frac{|\alpha_i|}{2}}\sum_{n_i=0}^{\infty}\frac{(\alpha_i)^{n_i}}{\sqrt{n_i!}}|n_i\rangle\right] \\ &= e^{-\frac{|\alpha|^2}{2}}\sum_{n_1,\dots,n_D=0}^{\infty}\frac{(\alpha_1)^{n_1}\cdots(\alpha_D)^{n_D}}{\sqrt{n_1!}\cdots\sqrt{n_D!}}|n_1, n_2, \dots, n_D\rangle \end{aligned} \tag{742}$$

with $|\alpha|^2 := |\alpha_1|^2 + \ldots + |\alpha_D|^2$.

Now we explain how the constraint C or the constraint operator $\hat{C}$, gets involved and how the physical coherent states are obtained via group averaging from the kinematical ones. In [64] they consider two cases. In the first case the kernel of the constraint operator is a subspace of the kinematical Hilbert space $\mathcal{H}_{\text{kin}}$. Therefore, it is assumed that $\hat{C}$ is self-adjoint and zero is a discrete point in its spectrum. Then the physical states are just a projection from the kinematical space $\mathcal{H}_{\text{kin}}$ to the physical subspace $\mathcal{H}_{\text{phy}}$. Under the condition that the 1-parameter group $\hat{U}(\lambda) = e^{-i\lambda\hat{C}}$ generated by $\hat{C}$ on $\mathcal{H}_{\text{kin}}$ provides a representation of U(1), this projection is given by the integral

$$|\Psi^{\text{phy}}\rangle = \frac{1}{\Lambda}\int\limits_0^{\Lambda} \mathrm{d}\lambda\, \hat{U}(\lambda)|\Psi\rangle \tag{743}$$

for any $|\Psi\rangle \in \mathcal{H}_{\text{kin}}$ and Λ such that $e^{-i\Lambda\hat{C}} = \hat{\mathbb{1}}$. Due to the circumstance that the physical coherent states are still elements of $\mathcal{H}_{\text{kin}}$ by construction, their scalar product can be calculated as

$$\langle\Psi^{\text{phy}}|\Phi^{\text{phy}}\rangle = \langle P\Psi|P\Phi\rangle = \langle P\Psi|\Phi\rangle = \frac{1}{\Lambda}\int\limits_0^{\Lambda} \mathrm{d}\lambda\, \langle e^{-i\lambda\hat{C}}\Psi|\Phi\rangle, \tag{744}$$

where P indicates the projection to the physical subspace. This is equivalent to a group averaging over U(1). As one can check, the resulting states are physical states in the sense that they satisfy $\hat{C}|\Psi^{\text{phy}}\rangle = 0$. The group averaging procedure in eq. (744) can also be carried over to cases where the constraint operator has no pure point spectrum, then $\mathcal{H}_{\text{phy}}$ is not a subspace of $\mathcal{H}_{\text{kin}}$ as discussed in [64]. In this second case one can still apply the group averaging projector on kinematical states which then involves an integral over the non-compact group $\mathbb{R}$ and becomes

$$|\Psi^{\text{phy}}\rangle = \frac{1}{K}\int\limits_{\mathbb{R}} \mathrm{d}\lambda\, \hat{U}(\lambda)|\Psi\rangle. \tag{745}$$

The resulting physical states are not normalizable with respect to the inner product in $\mathcal{H}_{\text{kin}}$ but can be understood as elements of the topological dual of a dense subspace of $\mathcal{H}_{\text{kin}}$ denoted by $\mathcal{S}$ on which elements of $\mathcal{S}^*$ act as distributions. The physical inner product is then defined as

$$\langle\Psi^{\text{phy}}|\Phi^{\text{phy}}\rangle = \frac{1}{K}\int\limits_{\mathbb{R}} \mathrm{d}\lambda\, \langle e^{-i\lambda\hat{C}}\Psi|\Phi\rangle, \tag{746}$$

with the corresponding norm given by

$$||\Psi^{\text{phy}}||^2 = \frac{1}{K}\int\limits_{\mathbb{R}} \mathrm{d}\lambda\, \langle e^{-i\lambda\hat{C}}\Psi|\Psi\rangle, \tag{747}$$

where the dense subset $\mathcal{S}$ is chosen such that Ψ^{phy} is a well defined distribution on $\mathcal{S}$, the norm of the physical states is finite and only vanishing if and only if Ψ^{phy} vanishes. For the toy model considered in this section we will need the second case, since the constraint operator has a continuous spectrum.

For the ***physical expectation value of an operator*** $\hat{\mathcal{O}}$ we introduce the notation

$$\langle\hat{\mathcal{O}}\rangle^{\text{phy}} := \frac{\langle\Psi^{\text{phy}}|\hat{\mathcal{O}}|\Psi^{\text{phy}}\rangle}{||\Psi^{\text{phy}}||^2}. \tag{748}$$

Since the standard harmonic oscillator is of this type, we are interested in ***quadratic constraints*** in the sense introduced in [64], where quadratic constraints of the following form were analyzed

$$C(q_i, p_i) := S_{ij} q_i q_j + K S_{ij} p_i p_j + A_{ij} q_i p_j - \Delta = 0, \tag{749}$$

here S_{ij} is a symmetric matrix, A_{ij} is an anti-symmetric matrix, K is a constant with dimension $\left[\ell^2/(\mathrm{Action})\right]^2$, Δ is a real constant and from now on we sum over double indices. The motivation for working with quadratic constraints in [64] was to formulate a toy model for gravity where the constraint needs to be zero in the classical theory. A quadratic constraint can be reformulated in terms of the holomorphic coordinates from eq. (740) which yields

$$C(q_i, p_i) := \kappa_{ij} \bar{z}_i z_j - \Delta = 0 \tag{750}$$

with a Hermitian matrix κ_{ij} and we set $\ell_i = \ell$ for all i. As a further simplification it is assumed that the original canonical coordinates are well adapted to the constraint C, such that κ_{ij}, reduces to a diagonal matrix and we define $\kappa_i := \kappa_{ii}$. Then the quantum constraint operator in natural ordering of $\hat{a}^\dagger$ and $\hat{a}$ becomes

$$\hat{C} = \kappa_j \hat{n}_j - \Delta \hat{\mathbb{1}} \tag{751}$$

and $\hat{n}_j := \hat{a}_j^\dagger \hat{a}_j$ is the jth number operator, where there is no summation over j in the definition of $\hat{n}_j$. The action of the operator $\hat{U}(\lambda) = e^{-i\lambda\hat{C}}$ on the kinematical coherent states $|\Psi_\alpha\rangle$ in eq. (742) can be calculated to be

$$e^{-i\lambda\hat{C}} |\Psi_\alpha\rangle = e^{i\lambda\Delta} |\Psi_{\alpha(\lambda)}\rangle \tag{752}$$

with $\alpha_j(\lambda) = e^{-i\lambda\kappa_j}\alpha_j$ and shows that again we obtain a coherent state whose peak compared to $|\Psi_\alpha\rangle$ is moved along the gauge orbit $\alpha(\lambda)$ generated by the constraint function C on the classical phase space Γ.

Now we want to apply the group averaging technique for quadratic constraints. In order to do so we need to ensure that $\hat{U}(\lambda)$ provides a representation of a group on $\mathcal{H}_{\mathrm{kin}}$. According to [64] the operator $\hat{U}(\lambda)$ provides a representation of U(1) if and only if for its action on the kinematical states we can find a real number Λ such that

$$e^{i\Lambda\Delta} = e^{-i\Lambda\kappa_i} = 1 \tag{753}$$

for all i. For the kind of quadratic constraints in eq. (750) and in case that $\hat{U}(\lambda)$ provides a representation of U(1), the physical Hilbert space $\mathcal{H}_{\mathrm{phy}}$, which is the kernel of the constraint operator $\hat{C}$, is also a subspace of $\mathcal{H}_{\mathrm{kin}}$ and we can apply the corresponding group averaging. As a consequence of the condition in eq. (753) all ratios κ_i/Λ and κ_i/κ_j have rational values. However, we want *all κ_i as well as Δ to be integers* which is achieved by multiplication of C by a constant and we chose $\Lambda = 2\pi$. Furthermore eq. (751) tells us that in order for $\hat{C}$ to have a non-trivial kernel κ_i and Λ need to satisfy the condition

$$\kappa_i n_i - \Delta = 0 \tag{754}$$

for some choice of integers $n_1, \ldots, n_D$. Additionally, for physical coherent states there is also a restrictions of the labels of the physical constrained coherent states, since at the physical level these classical labels are assumed to be consistent with the classical constraints. In the next section we want to apply these techniques to the fractional power constraint that we obtained after applying the dual Euler rescaling. For this purpose we have to generalize the analysis of the quadratic constraints from [64].

22.3 Physical Coherent States for Constraints with Fractional Hamiltonians

Large parts of this section are contained in the article [71]. Now we want to apply the techniques introduced in [64] and shortly summarized in section 22.2 to our fractional powers μ of the harmonic oscillator Hamiltonian which we shortly refer to as fractional Hamiltonians. Instead of considering the fractional Hamiltonians directly, we go over to the extended phase space as described in section 22.1 and consider a constraint of the form

$$C = p_t + H_{\text{ho}}^{\mu} = 0, \tag{755}$$

where p_t is the canonical conjugate momentum to a new time variable t and a constant of motion with respect to the fractional Hamiltonian in consideration. For fixed phase space coordinates q, p the temporal momentum p_t corresponds to the negative energy of the system, that is $p_t = -E^{(s)}$ with $E^{(s)} > 0$. Notice that for $\mu = 1$ this reduces to the case for the harmonic oscillator. Because of the general fractional power μ of the harmonic oscillator Hamiltonian the constraint in general might be difficult to handle. Therefore, we transform the constraint using the dual Euler rescaling to obtain an equivalent constraint as displayed in eq. (739) in section 22.1 which reads

$$\widetilde{C} = |p_t|^{\frac{1}{\mu}} - H_{\text{ho}} = |p_t|^{\frac{1}{\mu}} - \left(\frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 q^2\right) = |p_t|^{\frac{1}{\mu}} - \hbar\omega_0 \bar{z} z \approx 0 \tag{756}$$

for $z = \sqrt{\frac{m\omega_0}{2\hbar}}q + i\sqrt{\frac{1}{2\hbar m\omega_0}}p \in \mathbb{C}$. The kinematical Hilbert space of this model is $\mathcal{H}_{\text{kin}} = \mathcal{H}_1 \otimes \mathcal{H}_2 = L_2(\mathbb{R}, \mathrm{d}q) \otimes L_2(\mathbb{R}, \mathrm{d}p_t)$, where we use for both Hilbert spaces the standard Schrödinger representation, i.e. for the first one the occupation number representation and for the second one the momentum representation. The kinematical inner product for two kinematical states $|\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ and $|\Psi'\rangle = |\psi_1\rangle' \otimes |\psi_2'\rangle$ has the following form

$$\langle \Psi \mid \Psi' \rangle_{\text{kin}} = \langle \psi_1 \mid \psi_1' \rangle_{\mathcal{H}_1} \langle \psi_2 \mid \psi_2' \rangle_{\mathcal{H}_2}. \tag{757}$$

The constraint operator is then just given by

$$\hat{\widetilde{C}} = \hat{\mathbb{1}}_{\mathcal{H}_1} \otimes |\hat{p}_t|^{\frac{1}{\mu}} \hat{\mathbb{1}}_{\mathcal{H}_2} - \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right) \hat{\mathbb{1}}_{\mathcal{H}_1} \otimes \hat{\mathbb{1}}_{\mathcal{H}_2}. \tag{758}$$

As a first step we define kinematical coherent states whose expectation value of $\hat{\widetilde{C}}$ reproduces to lowest order in $\hbar$ the classical constraint. These kinematical coherent states can be obtained from a tensor product of the standard harmonic oscillator coherent states as follows

$$|\Psi_{\alpha,(t^0,p_t^0)}\rangle := |\Psi_\alpha\rangle \otimes |\Psi_{t^0,p_t^0}\rangle, \tag{759}$$

where $\alpha := \sqrt{\frac{m\omega_0}{2\hbar}}q_0 + i\sqrt{\frac{1}{2\hbar m\omega_0}}p_0$ and (t^0, p_t^0) are classical labels associated with the extended phase space. The explicit form of these states is given by

$$|\Psi_\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n}} |n\rangle \tag{760}$$

and

$$|\Psi_{t^0,p_t^0}\rangle = \int_{\mathbb{R}} \mathrm{d}p_t \Psi_{t^0,p_t^0}(p_t)|p_t\rangle = \int_{\mathbb{R}} \mathrm{d}p_t C_{t^0,p_t^0,\hbar} e^{-\frac{(p_t-p_t^0)^2}{2((\hbar\sigma)^\mu)^2}} e^{-\frac{i}{\hbar}p_t t^0}|p_t\rangle \tag{761}$$

with σ carrying units $[\sigma] = s^{-1}$ such that the arguments of all exponentials are dimensionless. If we define a similar dimensionless label α_t also for the temporal phase space coordinates, then σ will enter as $\alpha_t := \frac{\hbar}{\sqrt{2}(\hbar\sigma)^\mu}\left(\frac{(\hbar\sigma)^{2\mu}}{\hbar^2}t + \frac{i}{\hbar}p_t\right)$. The coherent state $|\Psi_\alpha\rangle$ is already normalized and we choose $C_{t^0,p_t^0,\hbar} = \frac{1}{(\pi^{\frac{1}{4}}\hbar\sigma)^\mu} e^{\frac{i}{\hbar}p_t^0 t^0} e^{-\frac{(p_t^0)^2}{2(\hbar\sigma)^{2\mu}}}$ such that also $|\Psi_{t^0,p_t^0}\rangle$ is normalized and thus $|\Psi_{\alpha,(t^0,p_t^0)}\rangle$ as well. The semiclassical expectation value of the constraint operator $\hat{\tilde{C}}$ can be computed as

$$\begin{aligned}\langle\Psi_{\alpha,(t^0,p_t^0)}|\,\hat{\tilde{C}}\,|\Psi_{\alpha,(t^0,p_t^0)}\rangle &= -\langle\Psi_\alpha|\,\hbar\omega_0(\hat{a}^\dagger\hat{a} + \frac{1}{2})\,|\Psi_\alpha\rangle + \langle\Psi_{t^0,p_t^0}|\,|\hat{p}_t|^{\frac{1}{\mu}}\,|\Psi_{t^0,p_t^0}\rangle \\ &= -\hbar\omega_0(\overline{\alpha}\alpha + \frac{1}{2}) + \langle\Psi_{t^0,p_t^0}|\,|\hat{p}_t|^{\frac{1}{\mu}}\,|\Psi_{t^0,p_t^0}\rangle.\end{aligned} \tag{762}$$

Using the techniques presented in [63], we can express the second semiclassical expectation value in terms of Kummer functions and obtain

$$\langle\Psi_{\alpha,(t^0,p_t^0)}|\,\hat{\tilde{C}}\,|\Psi_{\alpha,(t^0,p_t^0)}\rangle = -\frac{p_0^2}{2m} - \frac{m\omega_0^2q_0^2}{2} - \frac{\hbar\omega_0}{2} + \frac{\Gamma(\frac{\frac{1}{\mu}+1}{2})}{\sqrt{\pi}}\left((\hbar\sigma)^\mu\right)^{\frac{1}{\mu}}\,{}_1\mathrm{F}_1\left(-\frac{1}{2\mu}, \frac{1}{2}, -\frac{(p_t^0)^2}{(\hbar\sigma)^{2\mu}}\right), \tag{763}$$

here ${}_1\mathrm{F}_1(a, b, z)$ with $z \in \mathbb{C}$ denotes the Kummer function of the first kind also called the confluent hypergeometric function of the first kind. For more details on Kummer functions and particularly on how their Fourier transform can be used to obtain the above semiclassical expectation value we refer the reader to the work in [63]. As far as the semiclassical computations are concerned we are interested the sector where $\hbar$ is small compared to one, which allows us to express the semiclassical expectation value as an expansion in (fractional) powers of $\hbar$. The classical limit can then be obtained in the limit where we send $\hbar \to 0$. Consequently, in the case of the Kummer function we can use its asymptotic behaviour for large arguments which is well known. As shown in [63], the relevant asymptotic expansion for the semiclassical expectation value is given by

$$\langle\Psi_{t^0,p_t^0}|\,|\hat{p}_t|^{\frac{1}{\mu}}\,|\Psi_{t^0,p_t^0}\rangle \approx |p_t^0|^{\frac{1}{\mu}} \sum_{n=0}^{\infty} \frac{(-\frac{1}{2\mu})_n(\frac{\mu-1}{2\mu})_n}{n!}\left(\frac{(\hbar\sigma)^{2\mu}}{(p_t^0)^2}\right)^n, \tag{764}$$

where $(a)_n$ denotes the Pochhammer symbols also called raising factorials with $(a)_0 = 1, (a)_1 = a$ and $(a)_n = a(a+1)\cdots(a+n-1)$. Given these asymptotics of the Kummer function we obtain for the semilcassical expectation value of $\hat{\widetilde{C}}$

$$\begin{aligned}
&\langle\Psi_{\alpha,(t^0,p_t^0)}|\,\hat{\widetilde{C}}\,|\Psi_{\alpha,(t^0,p_t^0)}\rangle \qquad (765)\\
&\approx -\frac{p_0^2}{2m}-\frac{m\omega^2q_0^2}{2}-\frac{\hbar\omega_0}{2}+|p_t^0|^{\frac{1}{\mu}}\left(1-\frac{\frac{1}{\mu}(1-\frac{1}{\mu})}{4}\frac{(\hbar\sigma)^{2\mu}}{(p_t^0)^2}+o(\hbar^{4\mu})\right)\\
&=|p_t^0|^{\frac{1}{\mu}}-H_{\rm ho}+\hbar\frac{\omega_0}{2}-|p_t^0|^{\frac{1}{\mu}}\frac{\frac{1}{\mu}(1-\frac{1}{\mu})}{4}\frac{(\hbar\sigma)^{2\mu}}{(p_t^0)^2}+o(\hbar^{4\mu}),
\end{aligned}$$

where used $H_{\rm ho}=\frac{p_0^2}{2m}+\frac{m\omega_0^2q_0^2}{2}$. Hence, in the semiclassical limit $\hbar\to 0$ we recover the classical constraint $\widetilde{C}$

$$\lim_{\hbar\to 0}\langle\Psi_{\alpha,(t^0,p_t^0)}|\,\hat{\widetilde{C}}\,|\Psi_{\alpha,(t^0,p_t^0)}\rangle=|p_t^0|^{\frac{1}{\mu}}-H_{\rm ho}=\widetilde{C}. \qquad (766)$$

The point that we obtain in the limit $\hbar\to 0$ the correct classical expression confirms the theorem in [45] based on the Hamburger momentum problem by explicit computations in our toy model[3]. Due to the fact that using the techniques introduced in [63], we can also explicitly compute the higher than leading order terms. In this sense our results extend those in [45] concerning the formalism for non-polynomial operators. Note that for the special case that $\mu=\frac{1}{2n}$ with $n\in\mathbb{N}$ we have $\frac{1}{\mu}=2n$ and then the first argument of the Kummer function is $-n$ and in this case it can be expressed in terms of Hermite polynomials yielding for instance the expected semiclassical expectation value for p_t^2 for the choice of $n=1$. The rather unusual powers of $\hbar$ involving μ are due to the fact that in our case the unit of p_t is $[p_t]=J^\mu$, whereas for the spatial coordinates one uses the characteristic length of the harmonic oscillator $\ell:=\sqrt{\frac{\hbar}{m\omega}}$ to introduce dimensionless quantities and ℓ^2 is linearly in $\hbar$. For odd integers we have that p_t^n can also become negative but then even at the classical level due to the fact that $H_{\rm ho}>0$ the constraint $p_t^{\frac{1}{\mu}}-H_{\rm ho}\approx 0$ has no solutions and that is why we work with $|p_t|$ here. Note that this is similar to the situation for the reference matter models where on usually also restricts to certain parts of the full phase space by restricting the sign of the clock momentum, see for instance the discussion in [1, 23, 26, 63, 130, 167, 168].

The discussion so far was completely at the kinematical level, therefore we will apply the group averaging procedure to obtain physical coherent states along the lines of [64]. In our case the group averaging operator is given by

$$\hat{U}(\lambda)=e^{-\frac{i\lambda}{\hbar\omega_0}\left(\hat{\mathbb{1}}_{\mathcal{H}_1}\otimes|\hat{p}_t|^{\frac{1}{\mu}}\hat{\mathbb{1}}_{\mathcal{H}_2}-\hbar\omega_0(\hat{a}^\dagger\hat{a}+\frac{1}{2})\hat{\mathbb{1}}_{\mathcal{H}_1}\otimes\hat{\mathbb{1}}_{\mathcal{H}_2}\right)}=e^{i\lambda(\hat{n}+\frac{1}{2}\hat{\mathbb{1}}_{\mathcal{H}_1})}\otimes e^{-\frac{i\lambda}{\hbar\omega_0}|\hat{p}_t|^{\frac{1}{\mu}}\hat{\mathbb{1}}_{\mathcal{H}_2}}, \qquad (767)$$

where we used that $\hat{p}_t$ commutes with $\hat{H}_{\rm ho}$, rewrote $\hat{H}_{\rm ho}$ in terms of the number operator $\hat{n}=\hat{a}^\dagger\hat{a}$ and rescaled the constraint by $\hbar\omega_0$ in order to obtain a dimensionless quantity. Now we calculate the action of the unitary operator involved in the group averaging $\hat{U}(\lambda)=e^{-\frac{i\lambda}{\hbar\omega_0}\hat{\widetilde{C}}}$ on

[3] Note that there exist classical labels of the coherent states, for which the corresponding semiclassical expectation values might not satisfy the assumptions of the theorem.

the kinematical coherent state $\Psi_{\alpha,(t_0,p_t^0)}$ leading to

$$
\begin{aligned}
e^{-\frac{i\lambda}{\hbar\omega_0}\hat{\widehat{C}}}|\Psi_{\alpha,(t^0,p_t^0)}\rangle &= e^{i\lambda(\hat{n}+\frac{1}{2}\hat{\mathbb{1}}_{\mathcal{H}_1})}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle\otimes e^{-\frac{i\lambda}{\hbar\omega_0}|\hat{p}_t|^{\frac{1}{\mu}}\hat{\mathbb{1}}_{\mathcal{H}_2}}|\Psi_{t^0,p_t^0}\rangle \qquad (768)\\
&= e^{-\frac{|\alpha|^2}{2}}\int\limits_{\mathbb{R}}\mathrm{d}p_t\sum_{n=0}^{\infty}e^{i\lambda(n+\frac{1}{2})}\frac{\alpha^n}{\sqrt{n!}}|n\rangle\otimes e^{-\frac{i\lambda}{\hbar\omega_0}|p_t|^{\frac{1}{\mu}}}\Psi_{t^0,p_t^0}(p_t)|p_t\rangle\\
&= e^{-\frac{|\alpha|^2}{2}}\int\limits_{\mathbb{R}}\mathrm{d}p_t\sum_{n=0}^{\infty}e^{-\frac{i\lambda}{\hbar\omega_0}\left(|p_t|^{\frac{1}{\mu}}-\hbar\omega_0(n+\frac{1}{2})\right)}\frac{\alpha^n}{\sqrt{n!}}\Psi_{t^0,p_t^0}(p_t)|n\rangle\otimes|p_t\rangle,
\end{aligned}
$$

where $\Psi_{t^0,p_t^0}(p_t)$ denotes, as before, the standard coherent state in the momentum representation. Next we apply the group averaging to obtain physical coherent states which in our case will not be elements of $\mathcal{H}_{\text{kin}}$ but distribution on a dense subset $\mathcal{S}\subset\mathcal{H}_{\text{kin}}$, following closely the formalism in [64]. In addition we introduce a projection operator $\widehat{P}_{p_t<0}$ that projects on the negative part of the spectrum of $\hat{p}_t$ to ensure that the classical condition $p_t = -H^{\mu}_{\text{HO}}$ which requires $p_t < 0$ is also fulfilled at the quantum level. This projection operator can be implemented via $\widehat{P}_{p_t<0} := \mathbb{1}_{\mathcal{H}_1}\otimes\theta(-\hat{p}_t)$, where θ denotes the usual Heaviside function that vanishes if $p_t \geq 0$. Then we obtain the physical constrained coherent states as follows

$$
\begin{aligned}
|\Psi^{\text{phy}}_{\alpha,(t^0,p_t^0)}\rangle &= \frac{1}{K}\widehat{P}_{p_t<0}\int\limits_{\mathbb{R}}\mathrm{d}\lambda\,\hat{U}(\lambda)|\Psi_{\alpha,t^0,p_t^0)}\rangle = \frac{1}{K}\int\limits_{\mathbb{R}}\mathrm{d}\lambda\,\widehat{P}_{p_t<0}\hat{U}(\lambda)|\Psi_{\alpha,t^0,p_t^0)}\rangle \qquad (769)\\
&= \frac{e^{-\frac{|\alpha|^2}{2}}}{K}\int\limits_{\mathbb{R}}\mathrm{d}\lambda\int\limits_{\mathbb{R}}\mathrm{d}p_t\sum_{n=0}^{\infty}\theta(-p_t)e^{-\frac{i\lambda}{\hbar\omega_0}\left(|p_t|^{\frac{1}{\mu}}-\hbar\omega_0(n+\frac{1}{2})\right)}\frac{\alpha^n}{\sqrt{n!}}\Psi_{t^0,p_t^0}(p_t)|n\rangle\otimes|p_t\rangle\\
&= \frac{2\pi e^{-\frac{|\alpha|^2}{2}}}{K}\int\limits_{\mathbb{R}}\mathrm{d}p_t\sum_{n=0}^{\infty}\theta(-p_t)\delta\Big(\frac{|p_t|^{\frac{1}{\mu}}}{\hbar\omega_0}-(n+\frac{1}{2})\Big)\frac{\alpha^n}{\sqrt{n!}}\Psi_{t^0,p_t^0}(p_t)|n\rangle\otimes|p_t\rangle\\
&= \frac{2\pi e^{-\frac{|\alpha|^2}{2}}}{K}\int\limits_{\mathbb{R}}\mathrm{d}p_t\sum_{n=0}^{\infty}\hbar\omega_0\mu(\epsilon_n)^{\mu-1}\delta(p_t+\epsilon_n^{\mu})\frac{\alpha^n}{\sqrt{n!}}\Psi_{t^0,p_t^0}(p_t)|n\rangle\otimes|p_t\rangle,
\end{aligned}
$$

where we interchanged the order of the integration over λ with the summation and integration over p_t, used the definition of the Fourier transform of the delta function and defined $\epsilon_n := \hbar\omega_0(n+\frac{1}{2})$, $n\in\mathbb{N}_0$ in the last step. Here K is a real constant whose value can be chosen such that the resulting physical coherent states are normalized as done in eq. (772) below. Because the spectrum of $\hat{p}_t$ is the entire real line we have that even if we project to its negative part, that $\text{spec}(|\hat{p}_t|^{\frac{1}{\mu}})\cap\text{spec}(\hat{H}_{\text{HO}})\neq\emptyset$ and thus one obtains a non-trivial distribution after group averaging. Similarly to the example of the linear constraint in [64], where also a distributional physical coherent state is obtained, the result of the group averaging can be understood as the restriction of the kinematical coherent state to the constraint surface with an additional modification in the measure. The physical inner product can be explicitly computed and reads

$$
\begin{aligned}
\langle\,\Psi^{\text{phy}}_{\alpha,(t^0,p_t)}|\,\Psi^{\text{phy}}_{\beta,(t'^0,p'^0_t)}\rangle &= \frac{1}{K}\int\limits_{\mathbb{R}}\mathrm{d}\lambda\,\langle\widehat{P}_{p_t<0}\hat{U}(\lambda)\Psi_{\alpha,(t^0,p_t^0)}\,|\,\Psi_{\beta,(t'^0,p'^0_t)}\rangle \qquad (770)\\
&= \frac{2\pi\mu\hbar\omega_0}{K}e^{-\frac{|\alpha|^2+|\beta|^2}{2}}\sum_{n=0}^{\infty}\frac{(\overline{\alpha}\beta)^n}{n!}\epsilon_n^{\mu-1}\overline{\Psi}_{t^0,p_t^0}(-\epsilon_n^{\mu})\Psi_{t'^0,p'^0_t}(-\epsilon_n^{\mu}).
\end{aligned}
$$

$$
\begin{aligned}
||\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}||^2 &= \frac{1}{K}\int_{\mathbb{R}} \mathrm{d}\lambda\, \langle \hat{U}(\lambda)\Psi_\alpha|\Psi_\alpha\rangle = \frac{2\pi\mu\hbar\omega_0 e^{-|\alpha|^2}}{K}\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!}\epsilon_n^{\mu-1}|\Psi_{t^0,p_t^0}(-\epsilon_n^\mu)|^2 \\
&= \frac{2\pi\mu\hbar\omega_0 e^{-|\alpha|^2}}{K}\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!}\epsilon_n^{\mu-1}|\Psi_{t^0-p_t^0}(\epsilon_n^\mu)|^2 \\
&= \frac{2\pi e^{-|\alpha|^2}}{K}\sum_{n=0}^{\infty} c_{n;\mu}\frac{|\alpha|^{2n}}{n!}
\end{aligned}
\tag{771}
$$

here we used that for the absolute value we have $|\Psi_{t^0,p_t^0}(-\epsilon_n^\mu)|^2 = |\Psi_{t^0,-p_t^0}(\epsilon_n^\mu)|^2$ and in the last line we defined $c_{n;\mu} := \hbar\omega_0\mu\epsilon_n^{\mu-1}|\Psi_{t^0,-p_t^0}(\epsilon_n^\mu)|^2$. That the norm is finite is ensured by the fact that already $\frac{\alpha^n}{n!}$ is converging and due to the absolute value of the Gaussian evaluated at ϵ_n^μ for large values of n the sum involved in the norm is even stronger decreasing. We can obtain normalized physical coherent states by choosing $K = 2\pi$ and using the states

$$
\begin{aligned}
|\widetilde{\Psi}^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\rangle &:= \frac{|\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\rangle}{||\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}||} \\
&= \frac{e^{-\frac{|\alpha|^2}{2}}\int_{\mathbb{R}}\mathrm{d}p_t\sum_{n=0}^{\infty}\hbar\omega_0\mu\epsilon_n^{\mu-1}\delta(p_t+\epsilon_n^\mu)\frac{\alpha^n}{\sqrt{n!}}\Psi_{t^0,p_t^0}(p_t)|n\rangle\otimes|p_t\rangle}{\frac{2\pi e^{-|\alpha|^2}}{2\pi}\sum_{n=0}^{\infty}c_{n;\mu}\frac{|\alpha|^{2n}}{n!}}.
\end{aligned}
\tag{772}
$$

Then we have

$$
\begin{aligned}
\langle\widetilde{\Psi}^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\,|\,\widetilde{\Psi}^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\rangle &= e^{-|\alpha|^2}\sum_{n=0}^{\infty}\hbar\omega_0\mu\epsilon_n^{\mu-1}\frac{|\alpha|^{2n}}{n!}\frac{\int_{\mathbb{R}}\mathrm{d}p_t\,\delta(p_t+\epsilon_n^\mu)|\Psi_{t^0,p_t^0}|^2(p_t)}{||\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}||^2} \\
&= \frac{e^{-|\alpha|^2}\sum_{n=0}^{\infty}c_{n;\mu}\frac{|\alpha|^{2n}}{n!}}{e^{-|\alpha|^2}\sum_{n=0}^{\infty}c_{n;\mu}\frac{|\alpha|^{2n}}{n!}} = 1.
\end{aligned}
\tag{773}
$$

In case we compute the expectation value of the constraint $\hat{\widetilde{C}}$ with respect to the non-normalized physical coherent states $|\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\rangle$ setting $K = 2\pi$, we obtain

$$
\langle\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\,|\,\hat{\widetilde{C}}\,|\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\rangle = e^{-|\alpha|^2}\sum_{n=0}^{\infty}c_{n;\mu}\left(-\hbar\omega_0(n+\frac{1}{2})+(\epsilon_n^\mu)^{\frac{1}{\mu}}\right)\frac{|\alpha|^{2n}}{n!} = 0.
\tag{774}
$$

Next we compute the expectation value of the Dirac observable $\hat{H}_{\mathrm{ho}}$ in the physical coherent states and we end up with

$$
\frac{\langle\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\,|\hat{H}_{\mathrm{ho}}\,|\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\rangle}{||\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}||^2} = \frac{\sum_{n=0}^{\infty}c_{n;\mu}\hbar\omega_0(n+\frac{1}{2})\frac{|\alpha|^{2n}}{n!}}{\sum_{n=0}^{\infty}c_{n;\mu}\frac{|\alpha|^{2n}}{n!}} = \frac{\hbar\omega_0|\alpha|^2\sum_{n=0}^{\infty}c_{n+1;\mu}\frac{|\alpha|^{2n}}{n!}}{\sum_{n=0}^{\infty}c_{n;\mu}\frac{|\alpha|^{2n}}{n!}} + \frac{\hbar\omega_0}{2}.
\tag{775}
$$

As in [64, 163] we assume that the coherent states are peaked on the constraint surface. If we further use that $|p_t^0| = E_0^{(s)}$, where $E_0^{(s)}$ denotes the energy of the original system we started with and the 0-label was introduced here because the energy is determined by q_0, p_0, then we will have $\hbar\omega_0|\alpha|^2 = |p_t^0|^{\frac{1}{\mu}} = (E_0^{(s)})^{\frac{1}{\mu}}$ yielding to

$$\frac{\langle\Psi^{\text{phy}}_{\alpha,(t^0,p_t^0)}|\hat{H}_{\text{ho}}|\Psi^{\text{phy}}_{\alpha,(t^0,p_t^0)}\rangle}{||\Psi^{\text{phy}}_{\alpha,(t^0,p_t^0)}||^2} = (E_0^{(s)})^{\frac{1}{\mu}} \frac{\sum\limits_{n=0}^{\infty} c_{n+1;\mu}\frac{|\alpha|^{2n}}{n!}}{\sum\limits_{n=0}^{\infty} c_{n;\mu}\frac{|\alpha|^{2n}}{n!}} + \frac{\hbar\omega_0}{2}. \tag{776}$$

Although the zero point energy comes out exactly, in the case of the expectation value related to the classical energy $(E_0^{(s)})^{\frac{1}{\mu}}$ this is not like that. Here the corresponding contribution involves two sums one from the norm and a second one from the expectation value where the latter involves the coefficient $c_{n;\mu}$ with a shifted index by one. This carries over to a shift in $\epsilon^\mu_{n+1} = \left(\hbar\omega_0\left(n+\frac{3}{2}\right)\right)^\mu$ and to the absolute value of the Gaussian, thus we get

$$c_{n+1;\mu} = \hbar\omega_0\mu\left(\hbar\omega_0\left(n+\frac{3}{2}\right)\right)^{\mu-1}|\psi_{t^0,-p_t^0}(\epsilon^\mu_{n+1})|^2 \tag{777}$$

with

$$|\psi_{t^0,-p_t^0}(\epsilon^\mu_{n+1})|^2 = |C_{t^0,p_t^0,\hbar}|^2 e^{-\frac{1}{(\hbar\sigma)^{2\mu}}(\epsilon^\mu_{n+1}+p_t^0))^2}. \tag{778}$$

The sum of the squared norm in the denominator involves the same expression but with n and not $n+1$ in $c_{n+1;\mu}$. The label p_t^0 is the classical label of the coherent states associated with the temporal momentum. As discussed, on the classical constraint surface we can identify $\text{sgn}(p_t^0)p_t^0$ with the classical energy being equal to $E_0^{(s)}$, that is the μ-th fractional power of the energy of the classical harmonic oscillator. Due to the $\hbar$ in the denominator in the Gaussian it is narrowly peaked around the value of the classical energy $E_0^{(s)}$. Hence, the peak of the Gaussian with its fractional argument will be located at $E_0^{(s)}$. Because the classical energy is assumed to be large compared to the eigenvalues $\hbar\omega_0(n+\frac{1}{2})$ a reasonable choice for $|p_t^0| = E_0^{(s)}$ is a value that corresponds to large n in ϵ^μ_n. Consequently, the peak and hence the main contribution of this Gaussian with fractional argument will be at large values for n. Furthermore the $\frac{1}{n!}$ in each summand has the additional effect that the summands are further decreasing strongly with increasing n. Therefore, in the sum in the numerator we can replace $c_{n+1;\mu}$ by $c_{n;\mu}$ and the corrections due to this replacement are very tiny. The shift in $\epsilon^{\mu-1}_{n+1}$ involved in $c_{n+1;\mu}$ will be of minor order compared to the effects coming from the Gaussian and inverse factorial. If the absolute value of the Gaussian were absent, then to find a justification why large values of n will be most dominant would be difficult. So we realize that this is a specific feature of the physical coherent states. Assuming that we choose reasonable values for the classical energy that are sufficiently large compared to the energy eigenvalues of the harmonic oscillator Hamiltonian we obtain

$$\frac{\langle\Psi^{\text{phy}}_{\alpha,(t^0,p_t^0)}|\hat{H}_{\text{ho}}|\Psi^{\text{phy}}_{\alpha,(t^0,p_t^0)}\rangle}{||\Psi^{\text{phy}}_{\alpha,(t^0,p_t^0)}||^2} = (E_0^{(s)})^{\frac{1}{\mu}} + \frac{\hbar\omega_0}{2}. \tag{779}$$

Note that in [164] a similar strategy was considered. There the physical inner product still involves integrals and therefore variables were introduced that encode the deviation from the value around which the Gaussians in the coherent states are peaked. The resulting semiclassical expectation values were than written as an expansion consisting of a classical momentum variable and the width of the Gaussian. Despite that this seems to be more elaborate than in our case in the sense that they also include corrections around the classical value, the techniques they use cannot directly be carried over to our case, since we have no integrals involving Gaussians for the expectation value with respect to physical states left. Furthermore these corrections arise because functions in the integrand are Taylor expanded. More close to our case is the work done in [64] where among others semiclassical expectation values of generic observables being quadratic in annihilation and creation operators for constraints involving the number operator were discussed leading to a similar situation as in our case with two sums one from the norm in the denominator and the second one from the expectation values in the numerator. They considered the asymptotic values for these observables and assumed that one of the classical labels α_i is very large and tends to infinity. Given this, they could show that these two sums will drastically simplify, if they consider the dominant contributions yielding to the correct classical values of the quantum observables under these assumptions.

Considering now the result in eq. (779) we can solve this for the classical energy leading to an expression that involves fractional powers of the semiclassical expectation value of the harmonic oscillator Hamiltonian, namely

$$E_0^{(s)} = \left(\langle \Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)} | \hat{H}_{\mathrm{ho}} | \Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)} \rangle - \frac{\hbar\omega_0}{2} \right)^{\mu} . \tag{780}$$

We realize that in the limit $\hbar \to 0$ the μ-th power of the expectation value of $\hat{H}_{\mathrm{ho}}$ with respect to the normalized physical coherent states $|\widetilde{\Psi}^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}\rangle$ agrees with the classical energy $E_0^{(s)}$. If we had worked with the normal ordered Hamiltonian $:\hat{H}_{\mathrm{ho}}:$, as for instance done in [64], the $\hbar$ corrections due to the zero point energy would have even been absent. The reason why shifting the fractional power from the Hamiltonian to the temporal momentum works well here. The fractional power gets reintroduced in the final result by requiring that for physical coherent states their labels are peaked on the constraint surface which is a physically reasonable assumption and in this sense carries the fractional power of the operators over to the classical labels of the coherent states where they can be handled in a simpler manner. Let us compare the situation at the physical and kinematical level in this aspect. For this purpose we consider the Dirac observable $|p_t|^{\frac{1}{\mu}}$ which at the physical level coincides with the harmonic oscillator Hamiltonian. In the two cases we obtain for the semiclassical expectation values

$$\frac{\langle \Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)} | |\hat{p}_t|^{\frac{1}{\mu}} | \Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)} \rangle}{||\Psi^{\mathrm{phy}}_{\alpha,(t^0,p_t^0)}||^2} = \frac{\hbar\omega_0|\alpha|^2 \sum\limits_{n=0}^{\infty} c_{n+1;\mu} \frac{|\alpha|^{2n}}{n!}}{\sum\limits_{n=0}^{\infty} c_{n;\mu} \frac{|\alpha|^{2n}}{n!}} + \frac{\hbar\omega_0}{2} \approx \hbar\omega_0|\alpha|^2 + \frac{\hbar\omega_0}{2} \tag{781}$$

for large n and

$$\langle \widetilde{\Psi}_{\alpha,(t^0,p_t^0)} | |\hat{p}_t|^{\frac{1}{\mu}} | \widetilde{\Psi}_{\alpha,(t^0,p_t^0)} \rangle = \frac{\Gamma(\frac{\frac{1}{\mu}+1}{2})}{\sqrt{\pi}} \left((\hbar\sigma)^{2\mu}\right)^{\frac{1}{2\mu}} {}_1\mathrm{F}_1\left(-\frac{1}{2\mu}, \frac{1}{2}, -\frac{(p_t^0)^2}{(\hbar\sigma)^{2\mu}}\right). \tag{782}$$

Thus, even if we assume that the coherent state is peaked on the classical constraint surface, where we can use that $|p_t^0| = E_0^{(s)} = (\hbar\omega_0|\alpha|^2)^{\mu}$ and consider the expansion of the Kummer function for large arguments shown in eq. (765), we can observe that we obtain for the kinematical expectation values $\hbar$ corrections to $E_0^{(s)}$ that are not caused by the zero point energy of the harmonic oscillator but due to the in general fractional power associated with the temporal momentum. The underlying reason for this is that in the case of the physical coherent states due to the involved delta function the inner product is modified and hence the in general fractional powers of p_t need no longer to be integrated against the Gaussian of the coherent state which lead exactly to Kummer's function involved above in the kinematical case.

One can ask the question how the situation on the labels and the form of the states might change in case we apply reduced phase space quantization instead of Dirac quantization. As pointed out in [64] often the physical inner product can be identified with the inner product on the reduced phase space and we will discuss the situation for this model here. If we perform a reduced phase space quantization, we can identify the phase space variable t with our clock. Since the constraint $C = p_t + H^{\mu}_{\rm ho}$ is in deparametrized form, we can construct Dirac observables for q, p by choosing a gauge fixing condition $G = t - \tau$ and use the power series expansion introduced in [17, 19, 169]. In this simple model the power series can be written in closed form and we obtain for the Dirac observables

$$O_q(\tau) = \sum_{n=0}^{\infty} \frac{(-1)^n(\tau - t)^n}{n!}\{q, H^{\mu}_{\rm ho}\}_{(n)}, \quad O_p(\tau) = \sum_{n=0}^{\infty} \frac{(-1)^n(\tau - t)^n}{n!}\{p, H^{\mu}_{\rm ho}\}_{(n)}, \tag{783}$$

where $\{f, g\}_{(n)}$ denotes the iterated Poisson bracket with $\{f, g\}_{(0)} = f$ and $\{f, g\}_{(n)} = \{\{f, g\}_{(n-1)}, g\}$ with

$$\begin{aligned}
\{q, H^{\mu}_{\rm ho}\}_{(2n+1)} &= (-1)^n(\mu H^{\mu-1}_{\rm ho})^{2n+1}\omega_0^{2n+1}\frac{p}{m\omega_0}, \quad \{q, H^{\mu}_{\rm ho}\}_{(2n)} = (-1)^n(\mu H^{\mu-1}_{\rm ho})^{2n}\omega_0^{2n} q,\\
\{p, H^{\mu}_{\rm ho}\}_{(2n+1)} &= (-1)^{n+1}(\mu H^{\mu-1}_{\rm ho})^{2n+1}\omega_0^{2n+1} m\omega_0 q, \quad \{q, H^{\mu}_{\rm ho}\}_{(2n)} = (-1)^n(\mu H^{\mu-1}_{\rm ho})^{2n}\omega_0^{2n} p.
\end{aligned} \tag{784}$$

Reinserting this back into the observables in eq. (783) the closed form of these observables is given by

$$\begin{aligned}
O_q(\tau) &= \sin(\mu H^{\mu-1}_{\rm ho}\omega_0(t-\tau))q + \cos(\mu H^{\mu-1}_{\rm ho}\omega_0(t-\tau))\frac{p}{m\omega_0},\\
O_p(\tau) &= \sin(\mu H^{\mu-1}_{\rm ho}\omega_0(t-\tau))p - \cos(\mu H^{\mu-1}_{\rm ho}\omega_0(t-\tau))m\omega_0 q.
\end{aligned} \tag{785}$$

The algebra of these observables satisfies the standard canonical Poisson algebra, that is $\{O_q, O_p\} = 1$ and all remaining ones vanish. Given this explicit form of the observables we can explicitly show that indeed the physical $\mathrm{H}_{\rm phys} = H^{\mu}_{\rm ho}(O_q, O_p)$ generates their evolution. We have

$$\begin{aligned}
\frac{O_q(\tau)}{d\tau} &= -\mu H^{\mu-1}_{\rm ho}\omega_0\cos(\mu H^{\mu-1}_{\rm ho}\omega_0(t-\tau))q + \mu H^{\mu-1}_{\rm ho}\omega_0\sin(\mu H^{\mu-1}_{\rm ho}\omega_0(t-\tau))\frac{p}{m\omega_0},\\
&= \mu H^{\mu-1}_{\rm ho}\frac{O_p(\tau)}{m} = \frac{\partial H^{\mu}_{\rm ho}(O_q, O_p)}{\partial O_p} = \{O_q, H^{\mu}_{\rm ho}(O_q, O_p)\}
\end{aligned} \tag{786}$$

and

$$\begin{aligned}
\frac{dO_p(\tau)}{d\tau} &= -\mu H^{\mu-1}_{\rm ho}\omega_0\cos(\mu H^{\mu-1}_{\rm ho}\omega_0(t-\tau))p - \mu H^{\mu-1}_{\rm ho}\omega_0\sin(\mu H^{\mu-1}_{\rm ho}\omega_0(t-\tau))m\omega_0 q.\\
&= -\mu H^{\mu-1}_{\rm ho} m\omega_0^2 O_q = -\frac{\partial H^{\mu}_{\rm ho}(O_q, O_p)}{\partial O_q} = \{O_p, H^{\mu}_{\rm ho}(O_q, O_p)\}
\end{aligned} \tag{787}$$

The physical Hamiltonian is $\mathrm{H}_{\rm phys} = H^{\mu}_{\rm ho}(O_q, O_p)$ can be quantized using the standard Schrödinger representation and hence the reduced phase space is just $\mathcal{H}^{\rm red}_{\rm phys} = L_2(\mathbb{R}, \mathrm{dO}_q)$, where $\hat{O}_q$ acts by multiplication and $\hat{O}_p$ as a derivative operator. The quantization of the Hamiltonian allows to formulate the corresponding Heisenberg equations for $\hat{O}_q$ and $\hat{O}_p$ with the Hamiltonian operator $\hat{H}^{\mu}_{\rm ho}$. Going over to the Schrödinger picture, one obtains a standard Schrödinger-like equations with $\hat{H}^{\mu}_{\rm ho}$ as the involved Hamiltonian operator. Physical coherent states on the reduced physical Hilbert space can be constructed as

$$|\Psi_{O_\alpha}\rangle = e^{-\frac{|O_\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{O_\alpha^n}{\sqrt{n!}}|n\rangle \quad \text{with} \quad O_\alpha := \sqrt{\frac{m\omega_0}{2\hbar}} O_{q_0} + i\sqrt{\frac{1}{2\hbar m\omega_0}} O_{p_0}. \tag{788}$$

With respect to the inner product of $\mathcal{H}^{\rm red}_{\rm phys}$ these physical coherent states are normalized as one can easily see. The physical coherent states obtained via group averaging can be isometrically embedded into $\mathcal{H}^{\rm red}_{\rm phys}$ using the map

$$|n\rangle \rightarrow |\tilde{n}\rangle := \sqrt{c_{n;\mu}}|n\rangle \quad \text{with} \quad c_{n;\mu} := \hbar\omega_0\mu\epsilon_n^{\mu-1}|\Psi_{t^0,-p^0_t}(\epsilon^\mu_n)|^2, \quad K := 2\pi, \tag{789}$$

where we assumed, as mentioned above, that the constant $C_{t^0,p^0_t,\hbar}$ was chosen such that the coherent states $\Psi_{t^0,p_{t^0}}$ in $L_2(\mathbb{R}, {\rm d}p_t)$ were normalized. Using these rescaled states $|\tilde{n}\rangle$ in the reduced inner product yields the same result like for the physical coherent states in the physical inner product. Because in the reduced phase space any function involving the variables (t, p_t) can be expressed as a function of O_q, O_p only the expectation values for Dirac observables with respect to physical coherent states using group averaging and reduced phase space quantization agree under the identification $q_0 \rightarrow O_{q_0}, p_0 \rightarrow O_{p_0}$, compare also section 5.

Finally, let us briefly summarize the results obtained in this section. We used an Euler rescaling to rewrite the deparametrized constraint in the form that it involves the Hamiltonian linearly and the temporal momentum with some in general fractional power. We showed that using Kummer's confluent hypergeoemtric function the standard coherent states yield a good semiclassical approximation of the quantum constraint operator at the kinematical level. Then we applied group averaging to construct physical coherent states that are assumed to be peaked on the classical constraint surface. The latter allows to relate the absolute values of the labels of the coherent states to the energy of the system represented by the temporal momentum at the classical level. In this sense the coherent states intrinsically encode some dynamical properties via their labels and are beside the group averaging adapted to the constraint under consideration. Note that using coherent states that are peaked on the constraint surface was also crucial in [64] in order to obtain good semiclassical results for the operators corresponding to the classical Dirac observables. In our example discussed so far the coherent states are perfectly adapted to the Hamiltonian $\hat{H}_{\rm ho}$. As a consequence the relation between the classical energy $E_0^{(s)}$ and the semiclassical expectation value in (779) and (780) is very simple. For more complicated Hamiltonians one obtains a more complicated function of the coherent states labels α in which one then also replaces $\hbar\omega_0|\alpha|^2$ by $(E_0^{(s)})^{\frac{1}{\mu}}$. However, in order for the semiclassical states to be reasonable in lowest order in $\hbar$, we expect to obtain $(E_0^{(s)})^{\frac{1}{\mu}}$ plus possible further additional terms which then come with higher orders in $\hbar$ and can be interpreted as small corrections to the classical value. In order to test whether the semiclassical limit is correct, which corresponds to the limit $\hbar \rightarrow 0$, this method here can be useful but to work with the possible corrections involved could become problematic because the final step involves solving for $E_0^{(s)}$ which requires that the inverse function of the right hand side of (780) exists.

If we want to encode that the coherent states are peaked on the constraint surface directly into their labels, we can achieve this by implementing the corresponding restriction on the labels α. In our case we have $\hbar\omega_0|\alpha|^2 = (E_0^{(s)})^{\frac{1}{\mu}}$. Hence, we can label the coherent states with $\alpha = \frac{|E_0^{(s)}|^{\frac{1}{2\mu}}}{\sqrt{\hbar\omega_0}} e^{i\varphi}$. Then following the computations done above, we also end up with the results in (779) and (780). Although the states are adapted to the fractional power μ of the Hamiltonian by construction the label involves the inverse power $\frac{1}{\mu}$ which requires to solve for $E_0^{(s)}$. In the next section we want to consider the aspect that the labels of the coherent states carry some dynamical information from a different perspective and show that one can use coherent states for which the semiclassical expectation values involve directly the μth power of the classical energy and not the inverse power $\frac{1}{\mu}$.

In order to discuss temporal stability we use the notion of Klauder [33, 42]. For this one starts with a given Hamiltonian in the classical theory H and considers the corresponding operator $\hat{H}$ and some given set of coherent states $|\alpha;\delta\rangle$, where δ symbolizes all possible further labels next to the classical label α. One calls the states temporally stable under the evolution generated by $\hat{H}$ if

$$e^{-\frac{i}{\hbar}\hat{H}t}|\alpha(0);\delta\rangle = e^{i\theta(t)}|\alpha(t);\delta\rangle \tag{790}$$

where $\alpha(t)$ is a solution of $\frac{d\alpha(t)}{dt} = \{\alpha, H\}$ and we allow a physical irrelevant phase factor $e^{i\theta(t)}$. Thus temporal stability means here that the evolution of the state can (up to an irrelevant phase factor) be carried over to the classical labels of the coherent states. The standard example where this is given is the harmonic oscillator Hamiltonian $\hat{H}_{\rm ho}$ and the standard harmonic oscillator coherent states $|\alpha\rangle$. In this case we have $e^{-\frac{i}{\hbar}\hat{H}_{\rm ho}t}|\alpha(0)\rangle = e^{-i\hbar\omega_0 t}|\alpha(t)\rangle$.

As far as the dynamical stability under the harmonic oscillator Hamiltonian is concerned, we want to analyze the action of the evolution operator corresponding to the harmonic oscillator Hamiltonian on the coherent states $|\Psi^{\rm phy}_{\alpha,(t^0,p^0_t)}\rangle$. Using the fact that $|n\rangle$ are eigenstates of the Hamiltonian operator $\hat{H}_{\rm ho} = \hbar\omega_0(\hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{\mathbb{1}})$ with eigenvalues $E_n = \hbar\omega_0(n+\frac{1}{2})$, we obtain for the non-normalized physical coherent states $|\Psi^{\rm phy}_{\alpha(0),(t^0,p^0_t)}\rangle$ in eq. (769)

$$\begin{aligned}
&e^{-\frac{i}{\hbar}\hat{H}_{\rm ho}t}\otimes\mathbb{1}_{\mathcal{H}_2}|\Psi^{\rm phy}_{\alpha(0),(t^0,p^0_t)}\rangle \\
&= e^{-\frac{i}{\hbar}\hat{H}_{\rm ho}t}\otimes\mathbb{1}_{\mathcal{H}_2}\,\frac{2\pi e^{-\frac{|\alpha(0)|^2}{2}}}{K}\sum_{n=0}^{\infty}\hbar\omega_0\mu(\epsilon_n)^{\mu-1}\delta(p_t+\epsilon^\mu_n)\frac{\alpha^n(0)}{\sqrt{n!}}\Psi_{t^0,p^0_t}(p_t)|n\rangle\otimes|p_t\rangle \\
&= e^{-i\frac{\hbar\omega_0 t}{2}}\frac{2\pi e^{-\frac{|\alpha(0)|^2}{2}}}{K}\sum_{n=0}^{\infty}\hbar\omega_0\mu(\epsilon_n)^{\mu-1}\delta(p_t+\epsilon^\mu_n)\frac{(e^{-i\omega_0 t}\alpha(0))^n}{\sqrt{n!}}\Psi_{t^0,p^0_t}(p_t)|n\rangle\otimes|p_t\rangle \\
&= e^{-i\frac{\hbar\omega_0 t}{2}}|\Psi^{\rm phy}_{e^{-i\omega_0 t}\alpha(0),(t^0,p^0_t)}\rangle.
\end{aligned} \tag{791}$$

We see that up to a physically irrelevant phase factor the action of the Hamiltonian operator causes an additional rotation of the labels of the coherent states, which agrees with the classical evolution of the labels α under the evolution with respect to $H_{\rm ho}$. Hence, the physical coherent states $|\Psi^{\rm phy}_{\alpha,(t^0,p^0_t)}\rangle$ are temporally stable in the sense of Klauder as far as $\hat{H}_{\rm ho}$ as an effective substitute Hamiltonian operator for $\hat{H}^\mu_{\rm ho}$ is concerned. However, the states $|\Psi^{\rm phy}_{\alpha(0),(t^0,p^0_t)}\rangle$ are not temporally stable under the evolution generated by $\hat{H}^\mu_{\rm ho}$, since

$$\begin{aligned}
&e^{-\frac{i}{\hbar}\hat{H}^\mu_{\rm ho}\tilde{t}}\otimes\mathbb{1}_{\mathcal{H}_2}|\Psi^{\rm phy}_{\alpha(0),(t^0,p^0_t)}\rangle \\
&= \frac{2\pi e^{-\frac{|\alpha|^2}{2}}}{K}\sum_{n=0}^{\infty}\hbar\omega_0\mu(\epsilon_n)^{\mu-1}\delta(p_t+\epsilon^\mu_n)\frac{\alpha^n e^{-\frac{i}{\hbar}(\hbar\omega_0(n+\frac{1}{2}))^\mu\tilde{t}}}{\sqrt{n!}}\Psi_{t^0,p^0_t}(p_t)|n\rangle\otimes|p_t\rangle \\
&\neq e^{i\theta(\tilde{t})}|\Psi^{\rm phy}_{\alpha(\tilde{t}),(t^0,p^0_t)}\rangle,
\end{aligned} \tag{792}$$

where we used $\tilde{t}$ in order to emphasize that the dimension of t in the evolution operator of $\hat{H}_{\rm ho}$ and $\tilde{t}$ in the evolution operator of $\hat{H}^\mu_{\rm ho}$ are different as has been discussed in detail in section

22.1, which ensures that the argument of the exponential is dimensionless. The inequality in the last step was used because for the states the classical evolution to consider is $\frac{d\alpha}{dt} = \{\alpha, H^{\mu}_{\rm ho}\}$.

23 Coherent States for Fractional Poisson Distributions

Large parts of this section are contained in the article [71]. In section 22 we discussed how to apply the formalism developed in [64, 163] and combine it with the Euler rescaling in the context of an extended phase space to obtain coherent states which are, in the sense discussed above, adapted to square root Hamiltonians or more general fractional Hamiltonians. In this section we want to address the question of appropriate coherent states for fractional Hamiltonians from a different angle. As we saw in the last section 22 the physical coherent states differ from the kinematical ones by a restriction on their label set that is determined by the form of the constraint under consideration. Following this route here, we want to incorporate already into the construction of the coherent states that they should be well suited for fractional powers of the Hamiltonian. For this purpose we can restrict our discussion to the case of reduced phase space quantization and hence do not consider the degrees of freedom corresponding to t, p_t in the extended phase space here, since we have already shown in the last section that we obtain similar results for Dirac and reduced quantization for the example of fractional powers out of the harmonic oscillator that we consider here. In this case we quantize the algebra of Dirac observables shown in eq. (783) in the standard Schrödinger representation and their dynamics in the Heisenberg picture is generated by $\hat{H}^{\mu}_{\rm ho}$, the operator corresponding to the physical Hamiltonian of the Dirac observables.

There exist already preliminary work in the literature in the framework of so-called fractional Poisson distributions [65, 66], where in [66] generalized coherent states were constructed based on functions denoted as ***Mittag-Leffler functions*** which will be defined below in eq. (793). The work in [66] analyzes in detail the properties of these coherent states and presents a proof for their resolution of identity as well as temporal stability and we will briefly review the introduction of these states in section 23.1. As we will show in section 23.2 the proof presented in [66] is based on an incorrect assumption as far as the orthogonality of the angular part of the coherent states is considered. By generalizing the measure involved in the resolution of identity along the lines introduced in [170] we can correct this and introduce a slightly different set of coherent states that satisfies a resolution of identity. Furthermore the set of coherent states introduced here, has the property that the states are still eigenstates of the annihilation operator which is is not the case for the coherent states in [66].

23.1 Coherent States based on the Fractional Poisson Distribution

Before we introduce the generalized set of coherent states we briefly review the main results from [65, 66] because part of them can be seen as the motivation for introducing the generalized harmonic oscillator coherent states in this work. One of the main ideas in this construction is to obtain states that are no longer build from a Poisson distribution, like the standard harmonic oscillator coherent states but a more general probability distribution associated with the Mittag-Leffler function. This function can be understood as a generalization of the exponential function usually involved in the Poisson distribution. There exist several generalizations of the original Mittag-Leffler function which are encoded in additional parameters the function depends on. The ***original Mittag-Leffler function*** just depends on one parameter $\mu > 0$ and is given by

$$z \in \mathbb{C}, \quad z \mapsto E_{\mu}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\mu n + 1)}, \tag{793}$$

where Γ denotes the standard Gamma function with $\Gamma(z+1) = z\Gamma(z)$ and E_μ is an entire function. It can be understood as a kind of stretched exponential due to the Gamma function in the denominator. In the special case of $\mu = 1$ we have $\Gamma(n+1) = n!$ and then the Mittag-Leffler function E_μ becomes the usual exponential function. In this work we are interested in the parameter range $0 < \mu \leq 1$. The coherent states introduced in [66] are of the form

$$|\varsigma; \mu\rangle_{\mathrm{ML}} = \sum_{n=0}^{\infty} \frac{(\sqrt{\mu}\varsigma^\mu)^n}{\sqrt{n!}} \left(E_\mu^{(n)}(-\mu|\varsigma|^{2\mu})\right)^{\frac{1}{2}} |n\rangle, \quad 0 < \mu \leq 1, \tag{794}$$

where we introduced the label ML to emphasize that the states involve the Mittag-Leffler function and we introduced $\varsigma = \sqrt{\frac{m\omega_0}{2\hbar}} q_0 + i\sqrt{\frac{1}{2\hbar m\omega_0}} p_0$, where $E_\mu^{(n)}(-\mu|\varsigma|^{2\mu})$ denotes the n-th derivative of E_μ given by

$$E_\mu^{(n)}(-\mu|\varsigma|^{2\mu}) := \frac{d^n}{dz^n} E_\mu(z)\Big|_{z=-\mu|\varsigma|^{2\mu}}. \tag{795}$$

For the choice of $\mu = 1$ they reduce to the standard harmonic oscillator coherent states with the identification $\varsigma = \alpha$

$$\begin{aligned} |\alpha; 1\rangle_{\mathrm{ML}} &= \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \left(E_1^{(n)}(-|\alpha|^2)\right)^{\frac{1}{2}} |n\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \left(e^{-|\alpha|^2}\right)^{\frac{1}{2}} |n\rangle \\ &= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \end{aligned} \tag{796}$$

As shown in [66] the generalized coherent states in eq. (794) are normalized. Furthermore in [66] it is claimed that these coherent states satisfy a resolution of identity. However, the proof presented in [66] involves a mistake and we will discuss below how such mistake can be avoided by modifying the measure involved in the resolution of identity. This will then provide the basis for introducing a generalization of the harmonic oscillator coherent states that are better adapted to operators involving fractional powers.

As a further property in [66] it is discussed that these coherent states are stable under the dynamics of the harmonic oscillator Hamiltonian. However, here one has to differentiate depending on the notion of stability in consideration because temporal stability in the sense of Klauder [33], will only be given, if the action of the dynamical evolution operator (up to a complex phase) carries over to the labels ς of the coherent states, meaning that the labels follow exactly the classical time evolution. Although, the action of the evolution operator on the coherent states defined in [66] just causes a shift in the labels and hence maps again to another coherent state which means stability in the general sense discussed in section 21, this shift does not agree with the time evolution of the labels in the classical theory. We will discuss this issue in more detail below when we analyze the stability properties in detail.

Now the reason why nevertheless these states are interesting in the context of fractional Hamiltonians is that in these cases the expectation value of the number operator $\hat{n} = \hat{a}^\dagger\hat{a}$ is a fractional power of $|\varsigma|^2 = |\alpha|^2$, where the last equality is obtained by comparison of

$${}_{\mathrm{ML}}\langle\varsigma; \mu|\, \hat{a}^\dagger\hat{a}\, |\varsigma; \mu\rangle_{\mathrm{ML}} = \frac{\mu|\varsigma|^{2\mu}}{\Gamma(\mu+1)}, \tag{797}$$

with the expectation value $\langle\alpha|\, \hat{a}^\dagger\hat{a}\, |\alpha\rangle = |\alpha|^2$ for the standard coherent states which will again be recovered, if we set $\mu = 1$ in the general case. These properties look already interesting as far as fractional operators are considered, however due to the factor coming from the Gamma function, the semiclassical limit might be stretched as well and hence deviates from the correct expression by this factor. Moreover, a further differences of $|\varsigma;\mu\rangle_{\mathrm{ML}}$ compared to the standard coherent states $|\alpha\rangle$ is that the generalized states for $\mu \neq 1$ are no longer eigenstates of the annihilation operator $\hat{a}$. The reason for this is that the n-th derivative of the Mittag-Leffler function $E_\mu^{(n)}$ depends on the order of n and thus cannot just be pulled in front of the summation, as it is the case for the standard exponential, whose derivative for all orders of n involves again the exponential function only up to possible additional factors coming from inner derivative contributions. Furthermore, since $|\varsigma;\mu\rangle_{\mathrm{ML}}$ are no eigenstates of $\hat{a}$, these states are less suitable for other operators than the number operator which have more generic dependencies on $\hat{a}$ and $\hat{a}^\dagger$ such as for instance a polynomial one. Note that there exists a generalized annihilation operator of the form

$$\hat{a}_{(\mu)}|n\rangle = \sqrt{g(n;\mu)}|n-1\rangle \quad \text{with} \quad g(n;\mu) = \sqrt{\frac{nE_\mu^{(n-1)}(-\mu|\varsigma|^{2\mu})}{E_\mu^{(n)}(-\mu|\varsigma|^{2\mu})}} \tag{798}$$

for which $|\varsigma;\mu\rangle_{\mathrm{ML}}$ is an eigenstate with eigenvalue $\sqrt{\mu}\varsigma^\mu$. For the choice $\mu = 1$ the operator $\hat{a}_{(\mu)}$ becomes the standard annihilation operator because $g(n;1) = \sqrt{n}$. Also only for this choice the algebra of $\hat{a}_{(\mu)}$, $\hat{a}^\dagger_{(\mu)}$ and the identity operator satisfy the standard commutation relations, in general it is more complicated and given by

$$[\hat{a}_{(\mu)}, \hat{a}^\dagger_{(\mu)}]|n\rangle = \left(\frac{(n+1)E_\mu^{(n)}(-\mu|\varsigma|^{2\mu})}{E_\mu^{(n+1)}(-\mu|\varsigma|^{2\mu})} - \frac{n\, E_\mu^{(n-1)}(-\mu|\varsigma|^{2\mu})}{E_\mu^{(n)}(-\mu|\varsigma|^{2\mu})} \right) |n\rangle, \tag{799}$$

and even depends on the state $|n\rangle$. Here we used that $\hat{a}^\dagger_{(\mu)}|n\rangle = \sqrt{g(n+1;\mu)}|n+1\rangle$.

Given this, in the next section we want to discuss a different set of generalized coherent states which are also normalized, satisfy a resolution of identity but in addition are also eigenstates of the annihilation operator $\hat{a}$ with in general eigenvalues of fractional powers of α. These states are different from the ones described in [66], since they do not involve the general Mittag-Leffler function E_μ but the Mittag-Leffler function E_1 only which agrees with the exponential function. They can be understood as standard coherent states of the harmonic oscillator but with labels that have been adopted to the fractional Hamiltonian under consideration. The reason why we want to construct these states in the case of fractional powers of the Hamiltonian is that given these states we can consider the standard harmonic oscillator Hamiltonian as a kind of effective Hamiltonian for the computation of the semiclassical expectation values. This is the case because the coherent states are constructed in a way that they encode the properties of the the fractional operator.

23.2 Generalized Coherent States for Fractional Hamiltonians

The generalized coherent states that will be discussed in this section are given by

$$|\alpha;\mu\rangle = \sum_{n=0}^{\infty} \frac{(\alpha^\mu)^n}{\sqrt{n!}} e^{-\frac{1}{2}|\alpha|^{2\mu}}|n\rangle = \sum_{n=0}^{\infty} \frac{(\alpha^\mu)^n}{\sqrt{n!}} \left(E_1^{(n)}(-|\alpha|^{2\mu})\right)^{\frac{1}{2}} |n\rangle \tag{800}$$

for $0 < \mu \leq 1$ and we used that $E_1(z) = e^z$. We trivially rewrote $|\alpha;\mu\rangle$ in the last step only to make the relation to the states $|\varsigma;\mu\rangle_{\mathrm{ML}}$ in eq. (794) more transparent. Likewise to the states in eq. (794) these states depend on an additional parameter μ but their explicit dependence is different. Moreover, we keep the exponential function in the definition and do not consider the Mittag-Leffler function here. The latter ensures that these states are still eigenstates of the usual annihilation operator. If we compare the corresponding probability distributions corresponding to the states $|\varsigma;\mu\rangle_{\mathrm{ML}}$ from section 23.1 and $|\alpha;\mu\rangle$, we will obtain

$$P_\mu^{\varsigma,\mathrm{ML}}(n) := |\langle n|\varsigma;\mu\rangle_{\mathrm{ML}}|^2 = \frac{(\mu|\varsigma|^{2\mu})^n}{n!}\frac{d^n}{dz^n}E_\mu(z)\Big|_{z=-\mu|\varsigma|^{2\mu}} \tag{801}$$

and

$$P_\mu^{\alpha}(n) := |\langle n|\alpha;\mu\rangle|^2 = \frac{(|\alpha|^{2\mu})^n}{n!}e^{-|\alpha|^{2\mu}} = \frac{(|\alpha|^{2\mu})^n}{n!}\frac{d^n}{dz^n}E_1(z)\Big|_{z=-|\alpha|^{2\mu}}, \tag{802}$$

where we as above in eq. (800) rewrote $P_\mu^\alpha(n)$ in the last step only to show their exact relation to $P_\mu^\varsigma(n)$. As shown in [66] the probability distribution $P_\mu^\varsigma(n)$ has the mean value

$$\overline{n}_{\varsigma,\mathrm{ML}} = \sum_{n=0}^{\infty} nP_\mu^{\varsigma,\mathrm{ML}}(n) = \frac{\mu|\varsigma|^{2\mu}}{\Gamma(\mu+1)}. \tag{803}$$

Considering the action of the annihilation and creation operator as

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{804}$$

one can show that this is equal to [66]

$$\overline{n}_{\varsigma} = \sum_{n=0}^{\infty} nP_\mu^{\varsigma}(n) = \frac{\mu|\varsigma|^{2\mu}}{\Gamma(\mu+1)} = \langle\varsigma;\mu|\,\hat{a}^\dagger\hat{a}\,|\varsigma;\mu\rangle \tag{805}$$

which is the relevant form for our physical applications. If we perform the same computations for $P_\mu^\alpha(n)$ and the states $|\alpha;\mu\rangle$, we will end up with

$$\overline{n}_{\alpha} = \sum_{n=0}^{\infty} nP_\mu^{\alpha}(n) = |\alpha|^{2\mu} = \langle\alpha;\mu|\,\hat{a}^\dagger\hat{a}\,|\alpha;\mu\rangle. \tag{806}$$

Despite that the final results in eq. (805) and eq. (806) look similar, the way one obtains them is different. In the first case the states $|\varsigma;\mu\rangle_{\mathrm{ML}}$ are no eigenstates of $\hat{a}$ but if one computes the summation in eq. (805) one has to combine the sum over n with the sum over k involved in the derivatives of the Mittag-Leffler function and uses the binomial theorem. The latter absorbs one of the sums and the second runs over the power index of the binomial theorem. However, the arguments inside the bracket in the binomial theorem are just identical up to a sign so that the only non-vanishing contributions comes from the case where the power index is equal to zero, see [65, 66] for more details. The combination of the two sums is only possible at the level of expectation values because when we consider the action on an individual coherent state the sum over k is still inside a square root and thus cannot be combined with the outer sum over n.

On the other hand for $P_\mu^\alpha(n)$ we can use that $|\alpha;\mu\rangle$ is an eigenstate of $\hat{a}$, which can be easily shown by

$$\begin{aligned}\hat{a}|\alpha;\mu\rangle &= e^{-\frac{1}{2}|\alpha|^{2\mu}}\sum_{n=1}^{\infty}\frac{(\alpha^\mu)^n}{\sqrt{n!}}\sqrt{n}|n-1\rangle = e^{-\frac{1}{2}|\alpha|^{2\mu}}\sum_{n=0}^{\infty}\frac{(\alpha^\mu)^{n+1}}{\sqrt{n!}}|n\rangle \\ &= \alpha^\mu|\alpha;\mu\rangle.\end{aligned} \tag{807}$$

Hence the eigenvalue is just given by α^μ. Let us check that the states $|\alpha;\mu\rangle$ satisfy all three requirements: (i) normalization, (ii) satisfy a resolution of identity and (iii) are eigenstates of the annihilation operator $\hat{a}$, where the last one was already shown above.

The normalization can easily be shown by

$$(i)\,\langle\alpha;\mu\,|\,\alpha;\mu\rangle = \sum_{n=0}^{\infty} P_\mu^\alpha(n) = e^{-|\alpha|^{2\mu}} \sum_{n=0}^{\infty} \frac{(|\alpha|^{2\mu})^n}{n!} = e^{-|\alpha|^{2\mu}} e^{|\alpha|^{2\mu}} = 1. \tag{808}$$

In order that these states qualify as coherent states the continuity in the parameter α needs to be given, see [171]. This is trivially satisfied here because α is the usual coherent states label used for the harmonic oscillator coherent states. The usual overcompleteness relation for the harmonic oscillator coherent states generalizes to

$$\langle\alpha;\mu\,|\,\beta;\mu\rangle = \exp(-\frac{1}{2}\left(|\alpha|^{2\mu} + |\beta|^{2\mu} - 2(\alpha^*\beta)^\mu\right)),$$

that will yield the usual expression if we set $\mu = 1$.

As far as (ii) the resolution of identity is considered for the conventional harmonic oscillator coherent states we have

$$\int_{\mathbb{C}} \mathrm{d}^2\alpha\,|\alpha\rangle\langle\alpha| W_\mu(|\alpha|^2) = \hat{\mathbb{1}}, \quad \text{with} \quad W_\mu(|\alpha|^2) = \frac{1}{\pi} \tag{809}$$

where $\mathrm{d}^2\alpha = \mathrm{d}(\Re(\alpha)\mathrm{d}(\Im(\alpha))$. This can be proven by transforming $\alpha = \sqrt{\frac{m\omega_0}{2\hbar}}q_0 + i\sqrt{\frac{1}{2\hbar m\omega_0}}p_0$ to polar coordinates yielding $\alpha = \rho e^{i\phi}$ with $\rho := |\alpha|$ with $0 \le \rho < \infty$, $0 \le \phi < 2\pi$ and using that $\{e^{in\phi}\}_{n\in\mathbb{N}}$ is an orthonormal basis in $L_2([0,2\pi],\frac{d\phi}{2\pi})$. For the coherent states $|\alpha;\mu\rangle_{\mathrm{ML}}$ in [66] as well as the ones $|\alpha;\mu\rangle$ introduced in our work, we work with a fractional label α^μ and hence we have $\alpha^\mu = \rho^\mu e^{in\mu\phi}$. Thus, for $\mu \neq 1$ $\{e^{in\mu\phi}\}_{n\in\mathbb{N}}$ is no longer an orthonormal basis of $L_2([0,2\pi],\frac{d\phi}{2\pi})$. However, this seems to be have overseen in the proof presented in [66] which therefore cannot be performed in the way presented in [66] and yields to the incorrect conclusion that these states satisfy a resolution of identity. As we will show this issue can be circumvented by generalizing the measure that is involved in the resolution of identity along the lines introduced in [170] and for instance applied in [172] and will use this strategy to prove that the states $|\alpha;\mu\rangle$ satisfy a resolution of identity. For this purpose, as suggested in [170], we extend the polar coordinates to their covering space with the domains $0 \le \rho < \infty$ and $-\infty < \phi < \infty$ and consider a measure $\nu(\rho,\phi)$ defined by

$$\int \mathrm{d}\nu(\rho,\varphi;\mu)F(\rho,\phi) := \lim_{\Gamma\to\infty} \frac{1}{2\Gamma} \int_0^\infty \mathrm{d}\rho\, W_\mu(\rho^2) \int_{-\Gamma}^{\Gamma} \mathrm{d}\phi\, F(\rho,\phi), \tag{810}$$

where $W_\mu(\rho^2)$ is a still to be determined positive weight function. This yields

$$\begin{aligned}
&\int \mathrm{d}\nu(|\alpha|,\phi;\mu)\,|\alpha;\mu\rangle\langle\alpha;\mu| \\
&= \lim_{\Gamma\to\infty}\frac{1}{2\Gamma}\int\limits_0^\infty \mathrm{d}|\alpha|\,W_\mu(|\alpha|^2)\int\limits_{-\Gamma}^{\Gamma}\mathrm{d}\phi|\alpha|,\phi;\mu\rangle\langle|\alpha|,\phi;\mu| \\
&= \lim_{\Gamma\to\infty}\frac{1}{2\Gamma}\int\limits_{-\Gamma}^{\Gamma}\mathrm{d}\phi\int\limits_0^\infty \mathrm{d}\rho\sum_{n,m=0}^{\infty} e^{i\mu(n-m)\phi}\frac{\rho^{\mu(n+m)+1}}{\sqrt{n!}\sqrt{m!}}e^{-\rho^{2\mu}}W_\mu(\rho^2)|n\rangle\langle m| \\
&= \lim_{\Gamma\to\infty}\frac{1}{2\Gamma}\sum_{n,m=0}^{\infty}\int\limits_0^\infty \mathrm{d}\rho\,\frac{\rho^{\mu(n+m)+1}}{\sqrt{n!}\sqrt{m!}}e^{-\rho^{2\mu}}W_\mu(\rho^2)\int\limits_{-\Gamma}^{\Gamma}\mathrm{d}\phi\,e^{i(n-m)\mu\phi}|n\rangle\langle m|,
\end{aligned}$$

where in the last step we interchanged the order of summation and integration. Now we can use that $\{e^{is\phi}\}_{s\in\mathbb{R}}$ is an orthonormal basis in $L_2(\mathbb{R}_{\mathrm{Bohr}},\mu_{\mathrm{Bohr}})$ where the inner product of this Hilbert space reads $\langle f\,,\,g\rangle = \lim\limits_{\Gamma\to\infty}\frac{1}{2\Gamma}\int_{-\Gamma}^{\Gamma}\mathrm{d}\phi\overline{f}(\phi)g(\phi)$. Performing the integration over the angle ϕ we obtain

$$\begin{aligned}
&\int \mathrm{d}\nu(|\alpha|,\phi;\mu)\,|\alpha;\mu\rangle\langle\alpha;\mu| = \sum_{n=0}^{\infty}\int\limits_0^\infty \mathrm{d}\rho\,\frac{\rho^{2\mu n+1}}{n!}e^{-\rho^{2\mu}}W_\mu(\rho^2)|n\rangle\langle n| \\
&= \frac{1}{2}\sum_{n=0}^{\infty}\int\limits_0^\infty \mathrm{d}x\,\frac{x^{\mu n}}{n!}e^{-x^\mu}W_\mu(x)|n\rangle\langle n|,
\end{aligned}$$

where in the last step we used the variable substitution $x=\rho^2$. Now we apply a further change of variables and introduce $y=x^\mu$ with $dy=\mu x^{\mu-1}dx=\mu y y^{-\frac{1}{\mu}}dx$. This results in

$$\int\limits_{\mathbb{C}} \mathrm{d}^2\alpha\,|\alpha;\mu\rangle\langle\alpha;\mu|W_\mu(|\alpha|^2) = \frac{1}{2}\sum_{n=0}^{\infty}\frac{1}{n!}\int\limits_0^\infty \mathrm{d}y\,y^n e^{-y}\frac{\mu y^{\frac{1}{\mu}}}{y}W_\mu(y)|n\rangle\langle n|.$$

Now we choose the weight function to be

$$W_\mu(y) = \frac{2y}{\mu y^{\frac{1}{\mu}}} \quad\longrightarrow W_\mu(\rho^2) = \frac{2}{\mu}(\rho^2)^{\frac{\mu-1}{\mu}},$$

which is positive, i.e. $W_\mu(\rho^2)>0$, then we end up with

$$\begin{aligned}
(ii)\;&\int \mathrm{d}\nu(|\alpha|,\phi;\mu)\,|\alpha;\mu\rangle\langle\alpha;\mu| = \sum_{n=0}^{\infty}\frac{1}{n!}\int\limits_0^\infty \mathrm{d}y\,y^n e^{-y}|n\rangle\langle n| \qquad (811)\\
&= \sum_{n=0}^{\infty}\frac{\Gamma(n+1)}{n!}|n\rangle\langle n| = \sum_{n=0}^{\infty}|n\rangle\langle n| = \hat{\mathbb{1}}
\end{aligned}$$

and this proves the resolution of identity for the states $|\alpha;\mu\rangle$. For the special choice of $\mu=1$ their weight function reduces to $W_\mu(\rho^2)=2$ which is exactly the weight function one obtains for the standard harmonic oscillator coherent states in case one performs a similar generalization of the measure for the angular part as we did above.

Given the states $\langle \alpha; \mu \,|$ labeled by μ, let us discuss how we can use them as semiclassical states for operators involving fractional powers. We turn back to our example where the physical Hamiltonian on the reduced phase is given by H^{μ}_{ho}. Now in the quantum theory we consider as an integer power substitute for the Hamiltonian operator $\hat{H}^{\mu}_{\text{ho}}$, the operator

$$\widetilde{\hat{H}}_{\text{ho}} := (\hbar\omega_0)^{\mu-1}\hat{H}_{\text{ho}} = (\hbar\omega_0)^{\mu}\left(\hat{a}^{\dagger}\hat{a} + \frac{\hat{\mathbb{1}}}{2}\right). \tag{812}$$

Considering the generalized coherent states above for the semiclassical expectation value we obtain

$$\begin{aligned}\langle \alpha; \mu \,|\widetilde{\hat{H}}_{\text{ho}}\,|\alpha; \mu\rangle &= \langle \alpha; \mu \,|(\hbar\omega_0)^{\mu}\left(\hat{a}^{\dagger}\hat{a} + \frac{\hat{\mathbb{1}}}{2}\right)|\alpha; \mu\rangle \\ &= (\hbar\omega_0)^{\mu}|\alpha|^{2\mu} + \frac{(\hbar\omega_0)^{\mu}}{2} \\ &= E^{\mu}_0 + \frac{(\hbar\omega_0)^{\mu}}{2}.\end{aligned} \tag{813}$$

From the last line we immediately see that up to the zero point energy that vanishes in the $\hbar \to 0$ limit the expectation value of the substitute operator, which only involves integer powers of $\hat{H}_{\text{ho}}$, yields the correct classical limit in the zeroth order of $\hbar$. Following this route for different fractional powers of the harmonic oscillator Hamiltonian, we can always use $\hat{H}_{\text{ho}}$ as a substitute operator for $\hat{H}^{\mu}_{\text{ho}}$ supposed that we multiply $\hat{H}_{\text{ho}}$ with the appropriate fractional powers of $\hbar\omega_0$ for dimensional reasons. For the fluctuations we obtain with

$$\langle \alpha; \mu \,|(\widetilde{\hat{H}}_{\text{ho}})^2\,|\alpha; \mu\rangle = \langle \alpha; \mu \,|(\hbar\omega_0)^{2\mu}(\hat{a}^{\dagger}\hat{a}\hat{a}^{\dagger}\hat{a} + \hat{a}^{\dagger}\hat{a} + \frac{1}{4}\,|\alpha; \mu\rangle = (\hbar\omega_0)^{2\mu}(|\alpha|^{4\mu} + 2|\alpha|^{2\mu} + \frac{1}{4}) \tag{814}$$

the expected result

$$(\Delta\widetilde{\hat{H}}_{\text{ho}})^2 = (\hbar\omega_0)^{2\mu}|\alpha|^{2\mu} = (\hbar\omega_0)^{\mu}E^{\mu}_0. \tag{815}$$

These fluctuations come with a non-vanishing fractional power of $\hbar$ and are thus small compared to E_0 and vanish in the $\hbar \to 0$ limit.

If we use the coherent states introduced by Laskin for the same expectation values, as shown in [65], we will end up with

$${}_{\text{ML}}\langle \varsigma; \mu \,|\widetilde{\hat{H}}_{\text{ho}}\,|\varsigma; \mu\rangle_{\text{ML}} = (\hbar\omega_0)^{\mu}(\frac{\mu|\varsigma|^{2\mu}}{\Gamma(\mu+1)} + \frac{1}{2}) = \frac{\mu E^{\mu}_0}{\Gamma(\mu+1)} + \frac{(\hbar\omega_0)^{\mu}}{2} \tag{816}$$

showing that even in the lowest order of $\hbar$ we do not obtain the expected classical limit if $\mu \neq 1$. For the fluctuations following [65] we use that

$${}_{\text{ML}}\langle \varsigma; \mu \,|(\widetilde{\hat{H}}_{\text{ho}})^2\,|\varsigma; \mu\rangle_{\text{ML}} = 2(\hbar\omega_0)^{\mu}\frac{\mu E^{\mu}_0}{\Gamma(\mu+1)} + \left(\frac{\mu E^{\mu}_0}{\Gamma(\mu+1)}\right)^2\left(\frac{\sqrt{\pi}\Gamma(\mu+1)}{2^{2\mu-1}\Gamma(\mu+\frac{1}{2})}\right) + \frac{(\hbar\omega_0)^{2\mu}}{4} \tag{817}$$

and this leads to

$$(\Delta\widetilde{\hat{H}}_{\mathrm{ho}})^2_{\varsigma,\mathrm{ML}} = (\hbar\omega_0)^\mu \frac{\mu E_0^\mu}{\Gamma(\mu+1)} + \left(\frac{\mu E_0^\mu}{\Gamma(\mu+1)}\right)^2 \left(\frac{\sqrt{\pi}\Gamma(\mu+1)}{2^{2\mu-1}\Gamma(\mu+\frac{1}{2})} - 1\right), \tag{818}$$

where the label ς,ML should emphasize that these are the fluctuations associated with the coherent states based on the Mittag-Leffler functions. We find that these fluctuations have a more complicated structure than in the case of the generalized coherent states introduced in this work but also merge into the fluctuations of the standard harmonic oscillator coherent states if we choose $\mu = 1$ and use $\Gamma(\frac{3}{2}) = \frac{\sqrt{\pi}}{2}$. However, for $\mu \neq 1$ the fluctuations involve a contribution with zero power of $\hbar$ and therefore whether these fluctuations are small is not entirely determined by $\hbar$ but for the second term crucially depends on the value of E_0 being the only free parameter involved in the second term. This is a property which as far as the semiclassical properties of the coherent states $|\varsigma;\mu\rangle_{\mathrm{ML}}$ are concerned can become problematic if we aim at keeping fluctuations small in general.

We have already seen that the semiclassical states introduced in [66] based on the fractional Poisson distribution presented in [65] for $\mu \neq 1$ do not satisfy a resolution of identity, nor are they eigenstates of the annihilation operator. As the discussion above show they also do not yield the correct semiclassical limit for the Hamiltonian operator under consideration and further the size of the corresponding fluctuations can become large depending on the values of the classical labels of the coherent states. This leads to the conclusion that we would not consider these states as an appropriate set of semiclassical states for the operators of fractional power considered in this work. For the later purpose the generalized coherent states introduced here offer better functionality.

In [66] the temporal stability of the states $|\varsigma;\mu\rangle_{\mathrm{ML}}$ is analyzed and therefore we will briefly comment on this point also for the coherent states constructed in this section. For the discussion of the temporal stability here we use again the notion of Klauder [33, 42] and displayed in eq. (790). The evolution of the states $|\alpha;\mu\rangle$ in eq. (800) with respect to the harmonic oscillator yields

$$\begin{aligned} e^{-\frac{i}{\hbar}\hat{H}_{\mathrm{ho}}t}|\alpha(0);\mu\rangle &= e^{-\frac{1}{2}|\alpha(0)|^{2\mu}} \sum_{n=0}^{\infty} \frac{(\alpha^\mu(0))^n}{\sqrt{n!}} e^{-\frac{i}{\hbar}E_n t}|n\rangle \\ &= e^{-\frac{1}{2}|\alpha(0)|^{2\mu}} e^{-\frac{i}{2}\omega_0 t} \sum_{n=0}^{\infty} \frac{((e^{-\frac{i\omega_0 t}{\mu}}\alpha(0))^\mu)^n}{\sqrt{n!}}|n\rangle \\ &= e^{-\frac{i}{2}\omega_0 t}|\tilde{\alpha}(t);\mu\rangle \quad \text{with} \quad \tilde{\alpha}(t) := e^{-\frac{i\omega_0 t}{\mu}}\alpha(0). \end{aligned}$$

Again we have that up to a physically irrelevant phase factor the action of the Hamiltonian operator causes just a rotation of the labels of the coherent states. In the standard case $\mu = 1$, that is for states $|\alpha;1\rangle = |\alpha\rangle$, this change in the labels exactly corresponds to the classical equation of motion generated from the corresponding classical Hamiltonian. However, likewise to the states introduced in [66] for any other choice of μ the change in the labels is not in accordance with the classical equation of motion $\frac{d\alpha^\mu}{dt} = \{\alpha^\mu, H_{\mathrm{ho}}\}$ with corresponding solution $\alpha(t) = e^{-i\mu\omega_0 t}\alpha^\mu(0)$ and hence in the sense of Klauder [33, 42] one concludes that these states are not temporally stable under the evolution of the harmonic oscillator Hamiltonian. As we have discussed before in the physical Hilbert space a natural evolution operator is $\hat{H}^\mu_{\mathrm{ho}}$, the fractional harmonic oscillator Hamiltonian. These states are not temporally stable under the evolution generated by $\hat{H}^{\mu}_{\text{ho}}$ as we see by calculating

$$\begin{aligned} e^{-\frac{i}{\hbar}\hat{H}^{\mu}_{\text{ho}}\tilde{t}}|\alpha;\mu\rangle &= e^{-\frac{1}{2}|\alpha|^{2\mu}}\sum_{n=0}^{\infty}\frac{(\alpha^{\mu})^n e^{-\frac{i}{\hbar}(\hbar\omega_0(n+\frac{1}{2}))^{\mu}\tilde{t}}}{\sqrt{n!}}|n\rangle \\ &\neq e^{i\theta(t)}|\alpha(\tilde{t});\mu\rangle, \end{aligned} \tag{819}$$

again we used $\tilde{t}$ in order to emphasize that the dimension of t in the evolution operator of $\hat{H}_{\text{ho}}$ and $\tilde{t}$ in the evolution operator of $\hat{H}^{\mu}_{\text{ho}}$ are different, compare section 22.1. This ensures that the argument of the exponential is dimensionless. The inequality in the last step was used because for the states, which are labeled by α^{μ}, the classical evolution reads $\frac{d\alpha^{\mu}}{d\tilde{t}} = \{\alpha^{\mu}, H^{\mu}_{\text{ho}}\}$.

24 Conclusions

We started this part with section 14 where we stated our basic motivations and problems for the consideration of semiclassical states and we explained how coherent and semiclassical states can be defined. We considered the fundamental inspiring system of all coherent states construction principles: the harmonic oscillator. Next we discussed different ways to construct coherent or semiclassical states, where our main focus was on our toy model of a square root of a harmonic oscillator Hamiltonian, shortly denoted as square root Hamiltonian or a general fractional power thereof, shortly denoted as fractional Hamiltonian. As a result we found some ways to handle the square root Hamiltonian operator. Depending on the exact construction method, the resulting states satisfy, according to the definitions in section 14.1, more or less properties of semiclassical states but never all off them. Many of the constructions are based on the knowledge of the (energy) spectrum of the underlying Hamiltonian operator, like in sections 16 and 17. In our toy model approach this is easy because the underlying Hamiltonian operator is the harmonic oscillator Hamiltonian operator. However, in general this makes it difficult to transfer the results to the physical Hamiltonian operators in the Loop or Algebraic Quantum Gravity framework, since there the spectrum of the operator beneath the square root or beneath a fractional power is usually unknown. We tried to find some workarounds of that, in which one modifies the square root or fractional Hamiltonians at the classical level, compare sections 15 and 22, such that the fractional powers do not occur at the quantum level. These workarounds have the advantage that a knowledge of the spectrum of the underlying Hamiltonian operator is obsolete to construct semiclassical states, however one has to check whether the modified system still preserves properties of the original physical system in consideration. Our considerations about spectrum generating algebras and the stability of semiclassical states in section 20 and section 21, especially the definitions of the spectrum generating algebras (SGAs) in section 20.1 and the coherence breaking in in section 21.4.1, led us to the conclusion that for the square root or fractional Hamiltonian operator we should look for an algebra which is isomorphic to the Weyl-Heisenberg algebra or might consider the Weyl-Heisenberg algebra itself as a SGA for the square root or fractional Hamiltonian operator.

In section 15 we introduced a method we denote as the inverse Thiemann identity which uses the properties of the Poisson bracket to rewrite the square root at the classical level which leads to a harmonic oscillator Hamiltonian with a modified frequency. Afterwards when we went over to the quantum theory, we did this in a "semiclassical fashion" in the sense that we considered the classical energy of the square root Hamiltonian occurring in the modified frequency. We end up with an effective Hamiltonian which can be factorized in new annihilation and creation operators. The observation that these new annihilation and creation operators can also be obtained from a Bogoliubov transformation, brought us to the point that the eigenstates of the new annihilation and creation operators are given by squeezed states. However, by calculating the expectation value of the effective Hamiltonian in the squeezed state we came to the result that the squeezed states are not well-adapted to the effective Hamiltonian in a semiclassical sense, since they do not reproduce the classical value of the harmonic oscillator with modified frequency. What we took from this is that it seems a promising approach to avoid the square root at the classical level but we had to find a different way to go over to the quantum theory what was done in section 22.

An algebraically motivated approach was explored in section 16 by having a look at one possible generalizations of the Weyl-Heisenberg algebra with new annihilation $\hat{a}^-$ and creation operators $\hat{a}^+$. The new annihilation and creation operators can then be decomposed into the square root of the Hamiltonian operator expressed in terms of the number operator times the so-called phase operator or its adjoint operator. Eigenstates of this phase operator are the so-called phase states in [40] which are temporally stable states in the sense discussed there and displayed in section 16 . We were interested whether these states might serve as semiclassical states for the square root Hamiltonian, since the definitions of $\hat{a}^-$ and $\hat{a}^+$ originally contains a square root of an Hamiltonian operator, however the Hamiltonian operators themselves considered in [40] do not contain a square root. We saw that using the original definitions of $\hat{a}^-$ and $\hat{a}^+$ in case of our square root Hamiltonian led to contradictions, therefore we modified these definitions slightly by removing the square root of the Hamiltonian operator in the definitions of $\hat{a}^-$ and $\hat{a}^+$ to adapt to our square root Hamiltonian problem. This does not influence the definition of the phase operator and phase states themselves. The result of this was that the states are stable in the sense displayed in section 16 under the action of the square root Hamiltonian operator. However, they do neither reproduce the classical value of the Hamiltonian nor of the position or the momentum operator expressed in $\hat{a}^-$ and $\hat{a}^+$ when one calculates the expectation value of these operators in the phase states. Each of the expectation values even contains a diverging series. The only operator the phase states are by construction semiclassical states for is the phase operator. For these reasons they are not suitable for our purpose of finding semiclassical states for the square root Hamiltonian operator.

The starting point of section 17 are action-angle variables, the formulation of physical systems with discrete, nondegenerate energy spectra in these variables and the assumption that the classical action in these variables coincides with something Klauder calls the “quantum action”, see [33], which leads to the so-called action identity. Klauder et al. define a set of stable coherent states in the sense discussed in [33, 42] which satisfy this action identify, that is reassemble the classical value of the Hamiltonian in action-angle variables. We modified these states for our consideration of the square root Hamiltonian. On the first sight the result looks promising but there are several assumptions one has to make: first that the problem can be formulated in action-angle variables, second the convergence of a certain series which guarantees the normalization of the Klauder coherent states and third the existence of an n-th momentum of a given distribution. These are all things which might be not so easily to show and depend on the physical system in consideration.

In this part we considered the construction of complexifier coherent states in section 18 only from a theoretical point of view, since this method cannot be applied to our square root Hamiltonian problem. The complexifier coherent states are by construction adapted to integer powers of position and momentum operators and polynomials of them. Complexifier coherent states were applied in part IV in the context of semiclassical perturbation theory. Despite that the considerations about the stability of complexifier coherent states led to a common definition of stability for semiclassical states which we applied in section 21.

Section 19 introduces the algebraic construction method for semiclassical states and collects mathematical definitions about Lie groups and Lie algebras. The algebraic construction is based on the knowledge of the so-called spectrum generating algebra of a physical system. However, an algebra does not need to be a Lie algebra for the algebraic construction of coherent states.

Motivated by this, we investigated how to define spectrum generating algebras and how they can be obtained in section 20. We found that Lie algebras are preferable candidates for spectrum generating algebras due to their mathematical properties. Moreover, in section 20 we explored procedures which allow us to find some generators of a spectrum generating algebra but probably not all of them and each of these procedures can only be applied to a limited set of physical systems.

In section 21.1 we collected and compared the stability definitions for semiclassical states we have encountered so far. We observed that the one given in [31] is the most general one, however depending on which demands we have regarding the transformation of the labels of the semiclassical states with respect to the reproduction of the classical evolution, as it is investigated in section 22 and section 23, not always the suitable one. Nevertheless, we took the stability definition from [31] and combined it with the algebraic construction principle for coherent states for different types of algebras in section 21.2. In case of a Lie algebra, we found a closed formula for the temporally evolved states in section 21.2 and the expectation value of a generator of the spectrum generating Lie algebra in consideration in these states in section 21.3. To make section 21 round, we shortly collected some known results about stable systems in section 21.4 and especially about what kind of algebraic elements or more physically expressed terms appearing in an Hamiltonian operator cause the breaking of coherence in section 21.4.1.

Large parts of the conclusions for section 22 and section 23 are contained in the article [71]. The approach we analyzed in section 22 took as a starting point a constraint in deparametrized form $C = p_t + H^{\mu}_{\text{ho}}$ on an extended phase space with a corresponding physical Hamiltonian of the form H^{μ}_{ho}. Then we considered a canonical transformation on the extended phase space in the variables (t, p_t) as a kind of a so-called Euler rescaling which we introduced in section 22.1 that allowed us to rewrite the constraint in a form where a fractional power is no longer attached to H_{ho} but only to the temporal momentum p_t. This has the advantage that we could then show that the standard kinematical harmonic oscillator coherent states yield a good semiclassical approximation of the constraint operator by means of the technique of Kummer's functions introduced in [63]. Afterwards in section 22.3 we applied a group averaging procedure following [64] for the constraint with fractional temporal momentum and obtained the resulting physical coherent states and the physical inner product for this toy model. If we, as in [64, 163], require that the physical coherent states are peaked on the classical constraint surface, we can relate the semiclassical expectation value of $\hat{H}_{\text{ho}}$ with respect to physical coherent states to fractional powers of the classical energy involved in the classical constraint. Interestingly, compared to the standard harmonic oscillator coherent states, it is exactly the modification of the states that results from the group averaging procedure which leads to this property. For the case that an inverse function exists, which is the case in our simple toy model, we can relate fractional powers of this semiclassical expectation value to the classical energy, something that also happens in semiclassical perturbation theory. On the one hand this shows that the so obtained physical coherent states have by construction some restriction on their labels which encodes dynamical properties of the system. However, on the other hand following this route in the final step an inverse function needs to be applied in order to get how the classical energy is related to the semiclassical expectation value of the Hamiltonian H_{ho}. The existence of this inverse function can become an issue if the $\hbar$ corrections of the linear power of the operator under consideration depend in a complicated way on the classical labels of the coherent states. A way out of this can be to change the set of coherent states and choose a set for which the $\hbar$ corrections take a simpler form and then this strategy of computing semiclassical expectation values can still be applied. Furthermore we discuss in section 22.3 also how the results of the group averaging procedure and a reduced phase space quantization of the same model are related and show that we obtain equivalent results in both cases. Our results presented in this work extend the results of [64, 163] in the sense that there only linear or quadratic powers of the elementary operators were analyzed and here we considered fractional powers. We were able to extend their techniques to fractional powers by first shifting the fractional power from the Hamiltonian to the temporal momentum and second using the results in [63] that rely on the usage of Kummer's functions. At the end of section 23.2 we discuss the stability of the coherent states for fractional Hamiltonians constructed in this section.

In the approach in section 23.2 inspired by the coherent states based on a fractional Poisson distribution introduced in [66] we analyzed the question whether the labels of the coherent states can be adapted to Hamiltonians with fractional power. Although, the states in [66] yield fractional powers of the classical energy for the appropriately rescaled harmonic oscillator Hamiltonian a disadvantage of these states is that they are no longer eigenstates of the standard annihilation operator and they do not satisfy a resolution of identity as originally claimed in [66]. We showed how the proof can be modified and adapted to our generalized coherent states constructed in section 23.2. In contrast to the states in [66] the coherent states constructed in this article are still eigenstates of the standard annihilation operator. The reason why this is no longer the case for the Laskin states is that the exponential function usually involved in the standard harmonic oscillator coherent states is replaced by the so-called Mittag-Leffler function. Nevertheless, we can find a generalized annihilation operator which has the coherent state in [66] as an eigenstate. However, the algebra of these annihilation and creation operators does not reassemble the standard commutation relations and even depends on the number eigenstate. Moreover, in the semiclassical limit, that is the zeroth order of $\hbar$, the semiclassical expectation value yield not the expected classical result. This was one of the motivations for us to look for the generalized coherent states in section 23.2 which are still eigenstates of the annihilation operator but with an eigenvalue that involves fractional powers of the coherent states labels such as α^μ in our case. Since by construction the fractional power is already involved in the eigenvalues and the labels and hence the construction of the coherent states, we then used the usual harmonic oscillator Hamiltonian as a kind of effective operator to substitute the fractional power Hamiltonian. As shown in section 23.2 these states are in addition normalized and also satisfy a resolution of identity and the effective semiclassical computations yield good semiclassical properties. In contrast to the states in [66] they have the required classical limit. In addition we discuss the fluctuations of the states presented in 23.2 and the one from [66]. It turns out that due to the Mittag-Leffler function involved in the latter their fluctuations have a more complicated structure. Problematic here is that these fluctuations also involve a term that is zeroth order in $\hbar$, which is not the case for the generalized states in 23.1. As a consequence, the magnitude of these fluctuations is not mainly determined by $\hbar$ but depends on the value of the classical energy E_0. Only in the specific case where the fractional label μ is set to $\mu = 1$ this problematic term vanishes as expected because for $\mu = 1$ these states agree with the standard harmonic oscillator coherent states. At the end of section 23.2 we discuss the temporal stability of the coherent states considered in section 23.2.

Finally, let us comment on the question whether the two approaches discussed in section 22.3 and 23.2 can be generalized to more complicated situation than the toy model considered in this work. For the group averaging approach as long as we restrict to deparametrized models even for more complex Hamiltonian operators the constraints will be linearly in the temporal momentum, so the group averaging in the Hilbert space associated with the temporal degrees of freedom will have a similar effect. For instance in this work we considered coherent states based on the harmonic oscillator which can be also viewed as bosonic coherent states. There exist an extension to constrained fermionic systems introduced in [173]. We expect that for fermionic systems for which the dependence of the original Hamiltonian (without the fractional power) on the fermionic degrees of freedom is simple enough, the techniques of section 22.3 can be also carried over to those systems. However, in general the coherent states of the remaining degrees of freedom might not be so well adapted to the Hamiltonian as considered here and then the relation to the classical energy might no longer be so easily obtained. Nevertheless, any suitable coherent states should have the property that in lowest order of $\hbar$ one obtains the classical energy plus small corrections and thus as far as only a few corrections next to the leading order are considered this can be applicable tool. For more general applications it will depend on the specific form of the Hamiltonian. For instance the quantum mechanical analogue of the Hamiltonian one considers in deparametrized models of General Relativity are of the form $\hat{H} = (f_1(\hat{q})\hat{p}^{\mu_1} f_2(\hat{q}))^{\mu_2}$, where μ_1, μ_2 are fractional powers and f_1, f_2 are polynomial or exponential functions respectively. For the outer fractional power μ_2 the techniques presented in section 22.3 and 23.2 can be applicable in case the set of coherent states that one uses also approximates the function inside the outer fractional power, that is $f_1(\hat{q})\hat{p}^{\mu_1} f_2(\hat{q})$, semiclassically sufficiently well. For the inner fractional power μ_1 the strategy in section 22.3 is not applicable. Here techniques like semiclassical perturbation theory [4], the usage of Kummer's functions [63] or a choice of a different set of coherent states better adapted to the fractional operator than the standard harmonic oscillator ones along the lines of the discussion in section 23.2 will be preferred. As far as our second approach in section 23.2 is considered that works with coherent states involving fractional labels further more complicated applications need to be considered in order to understand their utility in full detail. We expect that these states can be useful for observables that are constructed from fractional powers of α and its complex conjugate as analyzed in this work. If we consider instead observables that involve fractional powers of q and p instead we guess that the method of using Kummer's functions in [63] are favoured. For more insights and a better understanding this needs to be investigated in future applications.

Part VI
Summary and Outlook

Part I presented the motivation for this work and part II gave an elaborate review on the state of the art of the canonical formulation of Loop Quantum Gravity (LQG). In this thesis we included our detailed conclusions concerning our research results at the end of part III, part IV and part V. Despite that we want to present a short overall summary and references to the conclusions of each part as well as an outlook for future research work at the very end of the thesis here.

In part III we examined reduced phase space quantization in contrast to Dirac quantization for four Klein-Gordon scalar fields in the context of LQG, respectively Algebraic Quantum Gravity (AQG), and as an alternative to the model discussed in [1] where one scalar field was used as reference matter for the Hamiltonian constraint, whereas the diffeomorphism constraints were handled using Dirac quantization, as explained in part II. The result shows that a naive extension of the Einstein-Hilbert action by the action of four Klein-Gordon scalar fields is not quantizable applying reduced phase space quantization and standard LQG techniques while for using Dirac quantization and standard LQG techniques it is. However, a further modification of the model by adding three more degrees of freedom additional to the four Klein-Gordon scalar fields makes it a quantizable model using reduced phase space quantization in the standard LQG or AQG framework. An interesting question for future work is to investigate whereas the different quantization procedures for the diffeomorphism constraints using reduced phase space quantization with additional scalar fields in this work and using Dirac quantization in [1] lead to different physical properties. This could be for instance analyzed in a simpler setting of spherically symmetric models where the diffeomorphism constraints simplify but still contribute. Moreover, one can further investigate the question for which kind of additional fields a reduced phase space quantization in the standard LQG framework is possible and how it is related to the corresponding quantum theory obtained via Dirac quantization. The detailed discussion can be found in the conclusions in section 10.

In part IV we tried to extend semiclassical perturbation theory within LQG or AQG to the class of physical Hamiltonian operators resulting from reduced phase space quantization. While in principle an extension is possible, we had to make two assumptions: first that the Hamiltonian operator is a self-adjoint operator which can usually be achieved by construction and second that the fluctuations of the approximation of the square of the Hamiltonian density in complexifier coherent states are sufficiently small. Both assumptions have to be checked for each physical Hamiltonian operator, respectively Hamiltonian density. This is not a simple task, since the spectra of the physical Hamiltonian operators as well as the expectation values of its Hamiltonian density in complexifier coherent states are usually unknown and therefore open to future research. Apart from that the expressions we obtain are getting technically quite involved and might require numerical tools to handle them. The detailed discussion can be found in the conclusions in section 13.

In part V we therefore explored an alternative perspective to perform a semiclassical analysis for the physical Hamiltonian operators by constructing new semiclassical states which are better adapted to the functional form of the physical Hamiltonian containing an outer square root. For this purpose as a first step towards this direction we work with a simple quantum mechanical toy model which is a fractional power out of the harmonic oscillator Hamiltonian (operator). We tried several approaches, for example: rewrite the outer square root on the classical level, consider the underlying algebra of the operator, work with canonical transformations of the coordinates, extend the phase space. Sometimes we also work with combinations of these ideas which actually leads us to a method to handle our toy model and also looks promising to be applicable to physical Hamiltonians which contain an outer square root. A future work is to actually apply this methods to different kinds of physical Hamiltonians containing an outer square root. The detailed discussion can be found in the conclusions in section 24 .

A Functional and Lie Derivative

Let us recall the definitions of the functional and the Lie derivative, see for example [9, 80].

Variation or Functional Derivative A.1. *Let ϕ belong to some manifold Φ of fields of certain type on a D dimensional manifold M (for example tensor fields with certain boundary conditions) and let $\delta\phi \in T_\phi(\Phi)$ be a tangential vector at $\phi \in \Phi$, known as **variation**. A functional $G : \Phi \to \mathbb{C}$ on Φ is said to be **functionally differentiable** at $\phi \in \Phi$ if there exists a continuous linear functional $(DG)_\phi$ on $T_\phi(\Phi)$ such that*

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} G[\phi + \lambda\delta\phi] \mid_{\lambda=0} = (DG)_\phi[\delta\phi]. \tag{820}$$

Usually $T_\phi(\Phi)$ is a space of test functions (smooth functions of compact support or rapid decrease, ...etc.). In these cases $(DG)_\phi$ can be written as a distribution

$$(DG)_\phi[\delta\phi] = \int\limits_M \mathrm{d}^D Y\, (DG)_\phi(Y) \bullet \delta\phi(Y), \tag{821}$$

where $\bullet$ means here the contraction with tensor or bundle indices. In physics it is common to call $(DG)_\phi$ the ***functional derivative*** of G at $\phi(Y)$ and to use the notation

$$(DG)_\phi(Y) =: \frac{\delta^{(D)} G[\phi]}{\delta\phi(Y)}. \tag{822}$$

Lie Derivative A.2. *Let M be a smooth manifold, p be a point in M, v be a smooth vector field on M and t be a smooth tensor field on M. Furthermore, let φ^v_t be a one-parameter family of a active diffeomorphisms generated by v (flow of v). Then the **Lie derivative** $\pounds_v t$ of any tensor field t along v is defined as*

$$(\pounds_v t)(p) := \frac{\mathrm{d}}{\mathrm{d}\lambda} \left((\varphi^v_\lambda)^* t \right)(p) \mid_{\lambda=0} \tag{823}$$

*with the **pull-back** denoted by * which means $\left((\varphi^v_\lambda)^* t \right)(p) = t\left(\varphi^v_\lambda(p)\right)$.*

B Observable Construction Formula

Large parts of this section have been published in [130]. If g is a scalar on phase space, e.g. some function $g : \chi \mapsto \mathbb{R}$ we claim

$$\{K_{\beta_1}, g(x)\}_{(n)} = \left[\beta_1^{j_1} ... \beta_1^{j_n} v_{j_1} ... v_{j_n} \cdot g\right](x) \tag{824}$$

with $v_j \cdot g(x) = \varphi^a_j g_a(x)$. In order to proof the claim it is of advantage to use that the vector fields mutually commute, that is $[v_j, v_k] = 0$ for all j, k. Using that spatial derivatives of δ^a_b vanish we get $0 = \partial_c(\delta^b_a) = \partial_c(\varphi^b_j \varphi^j_{,a})$ from which we can derive the useful identity

$$\varphi^b_{k,c} = -\varphi^b_j \varphi^j_{,ac} \varphi^a_k \tag{825}$$

The commutator of two vector fields yields

$$\begin{aligned} [v_j, v_k] &= \varphi^a_j \varphi^b_\ell \varphi^\ell_{,ac} \varphi^c_k \partial_b - \varphi^a_k \varphi^b_{j,a} \partial_b. \\ &= \varphi^a_j \varphi^b_\ell \varphi^\ell_{,ac} \varphi^c_k \partial_b - \varphi^a_k \varphi^b_{j,a} \partial_b \\ &= \varphi^b_{j,c} \varphi^c_k \partial_b - \varphi^a_k \varphi^b_{j,a} \partial_b \\ &= 0. \end{aligned} \tag{826}$$

We will proof the claim in eq. (824) by induction. For this purpose it is of advantage to express $\{K_{\beta_1}, \varphi^a_j(x)\}$ in terms of the vector fields v_j. We have

$$\begin{aligned}\{K_{\beta_1}, \varphi^a_j(x)\} &= -\varphi^a_k(x)\varphi^b_j(x)\{K_{\beta_1}, \varphi^k_{,b}(x)\} \\ &= -\varphi^a_k(x)\varphi^b_j(x)\int_\chi \mathrm{d}^3y\, \beta^\ell_1(y)\{c^{\mathrm{tot}}_\ell(y), \varphi^k_{,b}(x)\} \\ &= -\varphi^a_k(x)\varphi^b_j(x)\int_\chi \mathrm{d}^3y\, \beta^\ell_1(y)\{\pi_\ell(y) + h_\ell(y), \varphi^k_{,b}(x)\} \\ &= -\varphi^a_k(x)\varphi^b_j(x)\int_\chi \mathrm{d}^3y\, \beta^\ell_1(y)\{\pi_\ell(y), \varphi^k_{,b}(x)\} \\ &= -\varphi^a_k(x)\varphi^b_j(x)[\beta^k_1]_{,b}(x) \\ &= -\varphi^a_k[v_j \cdot \beta^k_1].\end{aligned} \tag{827}$$

Here we used in the fourth line that h_j is independent of the reference field momenta π_j. Now we can prove the claim by induction. For $n = 1$ we get

$$\{K_{\beta_1}, g(x)\}_{(1)} = [\beta^j_1 \varphi^a_j g_{,a}](x) = \beta^j_1 v_j \cdot g(x). \tag{828}$$

Suppose that the claim in eq. (824) is correct up to order n, then

$$\begin{aligned}\{K_{\beta_1}, g(x)\}_{(n+1)} &= \beta^{j_1}_1 ...\beta^{j_n}_1 \{K_{\beta_1}, v_{j_1}...v_{j_n} \cdot g(x)\} \\ &= \beta^{j_1}_1 ...\beta^{j_n}_1 \Big(v_{j_1}...v_{j_n}\{K_{\beta_1}, g(x)\} + \sum_{\ell=1}^{n} v_{j_1}...v_{j_{\ell-1}}\{K_{\beta_1}, \varphi^a_{j_\ell}\}\partial_a v_{j_{\ell+1}}...v_{j_n} \cdot g(x)\Big) \\ &= \beta^{j_1}_1 ...\beta^{j_n}_1 \Big(v_{j_1}...v_{j_n}\beta^{j_{n+1}}_1 v_{j_{n+1}} \cdot g(x) - \sum_{\ell=1}^{n} v_{j_1}...v_{j_{\ell-1}}v_{j_\ell}\beta^{j_{n+1}}_1 v_{j_{n+1}}v_{j_{\ell+1}}...v_{j_n} \cdot g(x)\Big) \\ &= \beta^{j_1}_1 ...\beta^{j_n}_1 \Big(v_{j_1}...v_{j_n}\beta^{j_{n+1}}_1 v_{j_{n+1}} \cdot g(x) - \sum_{\ell=1}^{n} v_{j_1}...v_{j_{\ell-1}}v_{j_\ell}\beta^{j_{n+1}}_1 v_{j_{\ell+1}}...v_{j_n}v_{j_{n+1}} \cdot g(x)\Big) \\ &= \beta^{j_1}_1 ...\beta^{j_n}_1 \Big(v_{j_1}...v_{j_n}\beta^{j_{n+1}}_1 v_{j_{n+1}} \cdot g(x) - \big(v_{j_1}...v_{j_n}\beta^{j_{n+1}}_1 - \beta^{j_{n+1}}_1 v_{j_1}...v_{j_n}\big)v_{j_{n+1}} \cdot g(x)\Big) \\ &= \beta^{j_1}_1 ...\beta^{j_{n+1}}_1 v_{j_1}...v_{j_{n+1}} \cdot g(x).\end{aligned} \tag{829}$$

In the third line we used equation (827), in the fourth line that the vector fields mutually commute and in the fifth line the Leibniz rule.
Hence the spatially diffeomorphism invariant quantity for g is given by

$$O^{(1)}_{g,\{\varphi^j\}}(\sigma) = g + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!}\big[\sigma^{j_1} - \varphi^{j_1}\big]\ldots\big[\sigma^{j_n} - \varphi^{j_n}\big]v_{j_1}...v_{j_n} \cdot g. \tag{830}$$

We have $v_j\varphi^k = \varphi^a_j\varphi^k_{,a} = \delta^k_j$. Using the abbreviation $\beta^j_1 := \sigma^j - \varphi^j$ we evaluate the action of v_k on the spatially diffeomorphism invariant quantity $O^{(1)}_g(\sigma)$

$$\begin{aligned}
v_k \cdot O^{(1)}_{g,\{\varphi^j\}}(\sigma) &= v_k \cdot g + v_k \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \beta^{j_1}_1 ... \beta^{j_n}_1 v_{j_1} ... v_{j_n} \cdot g \qquad (831)\\
&= v_k \cdot g + \sum_{n=1}^{\infty} \frac{n(-1)^n}{n!} \big[v_k \beta^j_1\big] \beta^{j_1}_1 ... \beta^{j_{n-1}}_1 v_{j_1} ... v_{j_{n-1}} \cdot g + \frac{(-1)^n}{n!} \beta^{j_1}_1 ... \beta^{j_n}_1 v_k v_{j_1} ... v_{j_n} \cdot g\\
&= v_k \cdot g + \big[v_k \beta^j_1\big] v_j \cdot g + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \beta^{j_1}_1 ... \beta^{j_n}_! \Big(\big[v_k \beta^j_1\big] v_j v_{j_1} ... v_{j_n} \cdot g + v_k v_{j_1} ... v_{j_n} \cdot g\Big)\\
&= v_k \cdot g + \big[v_k(\sigma^j - \delta^j_k)\big] v_j \cdot g + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \beta^{j_1}_1 ... \beta^{j_n}_1 \Big(\big[v_k \sigma^j - \delta^j_k\big] v_j v_{j_1} ... v_{j_n} \cdot g + v_k v_{j_1} ... v_{j_n} \cdot g\Big)\\
&= \big[v_k \sigma^j\big] v_j \cdot g + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \beta^{j_1}_1 ... \beta^{j_n}_1 \big[v_k \sigma^j\big] v_j v_{j_1} ... v_{j_n} \cdot g\\
&= \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \beta^{j_1}_1 ... \beta^{j_n}_1 \big[v_k \sigma^j\big] v_j v_{j_1} ... v_{j_n} \cdot g.
\end{aligned}$$

We realize that for constant $\sigma^j(x)$ the expression $v_k \cdot O^{(1)}_{g,\{\varphi^j\}}(\sigma)$ vanishes meaning that $O^{(1)}_{g,\{\varphi^j\}}(\sigma)$ does not depend on x at all as expected for a spatially diffeomorphism invariant quantity. Consequently we have the freedom to choose any x in the expression for $Og,\{\varphi^j\}^{(1)}(\sigma)$. A convenient choice for which $O^{(1)}_{g,\{\varphi^j\}}(\sigma)$ extremely simplifies is to choose x_σ such that $\varphi^j(x_\sigma) = \sigma^j$, since then only the $n = 0$ term in the whole summation survives. This requires that φ^j is invertible for $j = 1, 2, 3$ which is true because in order that φ^j qualifies as a good reference field we have to assume that φ^j are diffeomorphisms. For a scalar g on χ we therefore obtain the following explicit integral representation for the spatially diffeomorphism invariant expression

$$O^{(1)}_{g,\{\varphi^j\}}(\sigma) = \int_\chi \mathrm{d}^3x \,\big|\det(\partial\varphi^j/\partial_x)\big| \delta(\varphi^j(x), \sigma^j) g(x). \qquad (832)$$

C Comparison Reduced Model with Gauge Fixed Model

Large parts of this section have been published in [130]. In this section we want to compare the reduced generalized four scalar field model with its associated gauge fixed model. In case that we start on the partially reduced phase space with respect to the second class constraints (c^{jj}, Λ^{jj}), then the four gauge fixing conditions associated with the Hamiltonian and spatial diffeomorphism constraints read

$$G^0 = \tau^0 - \varphi^0 \quad G^j = \sigma^j - \varphi^j. \qquad (833)$$

Similar to the Brown-Kuchař dust model in [26] we assume that $\tau^0 = \tau^0(t)$ does not depend on the spatial coordinates and we assume σ^j to depend on the spatial coordinates only. Considering this and the form of the Hamiltonian and spatially diffeomorphism constraint on the partially reduced phase space the stability requirement for the gauge fixing conditions yields

$$\begin{aligned}
\text{(i)} \quad \frac{dG^0}{dt} &\overset{!}{\approx} 0 = \frac{\partial \tau^0}{\partial t} - \frac{n\pi_0}{\sqrt{q}} - n^a \varphi^0_{,a}, \\
\text{(ii)} \quad \frac{dG^j}{dt} &\overset{!}{\approx} 0 = -n\sqrt{q^{cd}\varphi^j_{,c}\varphi^j_{,d}} - n^a \varphi^j_{,a}.
\end{aligned} \tag{834}$$

The lapse function and shift vector induced by this kind of choice for the gauge fixing are given by

$$\begin{aligned}
n &\approx \frac{\partial \tau^0}{\partial t}\left(-\frac{h}{\sqrt{q}} - \varphi^0_{,a}\sum_{j=1}^{3}\varphi^a_j\sqrt{q^{cd}\varphi^j_{,c}\varphi^j_{,d}}\right)^{-1}, \\
n^a &\approx -\frac{\partial \tau^0}{\partial t}\frac{\sum\limits_{j=1}^{3}\left(\varphi^a_j\sqrt{q}\sqrt{q^{cd}\varphi^j_{,c}\varphi^j_{,d}}\right)}{\left(-h - \varphi^0_{,a}\sum\limits_{j=1}^{3}\left(\varphi^a_j\sqrt{q}\sqrt{q^{cd}\varphi^j_{,c}\varphi^j_{,d}}\right)\right)},
\end{aligned} \tag{835}$$

where we used that $\pi_0 \approx -h$. At the observable level these weak equalities simplify to

$$\begin{aligned}
O_{n,\{\varphi^0,\varphi^j\}} &= -\frac{\sqrt{Q}}{h(Q_{jk},P^{jk})} =: N(Q,P) \\
O_{n^a,\{\varphi^0,\varphi^j\}} &= \frac{1}{h(Q_{jk},P^{jk})}\sum_{j=1}^{3}\sqrt{Q}\sqrt{Q^{jj}}\delta^k_j =: N^k(Q,P)
\end{aligned} \tag{836}$$

with

$$h(Q_{jk},P^{jk}) := \sqrt{-2\sqrt{Q}C^{\rm geo} + 2\sqrt{Q}\sum_{j=1}^{3}\sqrt{Q^{jj}C^{\rm geo}_jC^{\rm geo}_j}}. \tag{837}$$

Let us denote the corresponding quantities in the gauge fixed theory by $n_0(q,p)$, $n^k_0(q,p)$ and $h(q,p)$ respectively whose explicit form is given by

$$\begin{aligned}
n_0(q,p) &= -\frac{\sqrt{q}}{h(q,p)} \\
n^k_0(q,p) &= \frac{1}{h(q,p)}\sum_{j=1}^{3}\sqrt{q}\sqrt{q^{jj}}\delta^k_j \\
h(q,p) &= \sqrt{-2\sqrt{q}c^{\rm geo} + 2\sqrt{q}\sum_{j=1}^{3}\sqrt{q^{jj}c^{\rm geo}_jc^{\rm geo}_j}}
\end{aligned} \tag{838}$$

This result is also consistent with the condition following from equation (350) for the gauge fixing chosen above. Given this we obtain for the dynamics of a function f that does not depend on the clock degrees of freedom in the gauge fixed theory:

$$\begin{aligned}
\frac{df}{d\tau} &= \left(\frac{\partial\tau^0}{\partial t}\right)^{-1}\frac{df}{dt}\Big|_{G^J=0,c=c_k=0,n=n_0,n^k=n_0^k}\\
&= \left(\frac{\partial\tau^0}{\partial t}\right)^{-1}\int d^3y\left(n_0(q,p)\{f,c^{\rm tot}(y)\}\Big|_{G^J=0,c=c_k=0}+n_0^k(q,p)\{f,c_k^{\rm tot}(y)\}\Big|_{G^J=0,c=c_k=0}\right)\\
&= \int \mathrm{d}^3y\left(-\frac{\sqrt{q}(y)}{h(q,p)}\{f,c^{\rm tot}(y)\}\Big|_{G^J=0,c=c_k=0}+\frac{1}{h(q,p)}\sum_{j=1}^3\sqrt{q}\sqrt{q^{jj}}(y)\delta_j^k\{f,c_k^{\rm tot}(y)\}\Big|_{G^J=0,c=c_k=0}\right)\\
&\approx \int \mathrm{d}^3y\,\frac{1}{2h(q,p)}\left(\{f,-2\sqrt{q}c^{\rm tot}(y)\}\Big|_{G^J=0,c=c_k=0}+\{f,\sum_{j=1}^3 2\sqrt{q}\sqrt{q^{jj}}(y)\delta_j^k c_k^{\rm tot}(y)\}\Big|_{G^J=0,c=c_k=0}\right)\\
&= \int \mathrm{d}^3y\,\frac{1}{2h(q,p)}\left(\{f,-2\sqrt{q}c^{\rm geo}(y)\}+\{f,\sum_{j=1}^3 2\sqrt{q}\sqrt{q^{jj}}\delta_j^k c_k^{\rm geo}(y)\}\right)\\
&= \int \mathrm{d}^3y\,\frac{1}{2h(q,p)}\left(\{f,-2\sqrt{q}c^{\rm geo}(y)+\sum_{j=1}^3 2\sqrt{q}\sqrt{q^{jj}}\delta_j^k c_k^{\rm geo}(y)\}\right)\\
&= \int \mathrm{d}^3y\,\frac{1}{2h(q,p)}\left(\{f,-2\sqrt{q}c^{\rm geo}(y)+\sum_{j=1}^3 2\sqrt{q}\sqrt{q^{jj}c_j^{\rm geo}c_j^{\rm geo}}(y)\}\right)\\
&= \int \mathrm{d}^3y\left(\{f,\sqrt{-2\sqrt{q}c^{\rm geo}(y)+\sum_{j=1}^3 2\sqrt{q}\sqrt{q^{jj}c_j^{\rm geo}c_j^{\rm geo}}(y)}\}\right)\\
&= \{f,\int \mathrm{d}^3y\,h(q,p)(y)\}\\
&= \{f,H^{\rm GF}\}
\end{aligned}\tag{839}$$

with gauge fixed Hamiltonian

$$H^{\rm GF}:=\int \mathrm{d}^3y\,h(q,p)(y).$$

We realize that the dynamics of the observables and the dynamics of the gauge fixed theory are identical.

D Calculations Generalized Model Four K.-G. Scalar Fields

D.1 Constraint Stability Analysis

In the following we need to perform the constraint analysis in order to check whether the primary constraints are stable under time evolution with respect to $H_{\rm primary}$ or not. The non-vanishing

Poisson brackets on the phase space are given by

$$\begin{aligned}
\{q_{cd}(x), p^{ab}(y)\} &= \kappa\delta^a_{(c}\delta^b_{d)}\delta^{(3)}(x,y), \\
\{n(x), p(y)\} &= \delta^{(3)}(x,y), \\
\{n^a(x), p_b(y)\} &= \delta^a_b\delta^{(3)}(x,y), \\
\{\varphi^0(x), \pi_0(y)\} &= \delta^{(3)}(x,y), \\
\{\varphi^j(x), \pi_k(y)\} &= \delta^j_k\delta^{(3)}(x,y), \\
\{M_{ij}(x), \Pi^{k\ell}(y)\} &= \delta^k_{(i}\delta^\ell_{j)}\delta^{(3)}(x,y).
\end{aligned} \tag{840}$$

The primary constraints are given by

$$z := p, \quad z_a := p_a, \quad \Phi_j := \pi_j - \sqrt{q}M_{jk}\varphi^k_n, \quad \Pi^{ij} := \Lambda^{ij}, \quad c^{\mathrm{tot},0} := c^{\mathrm{geo}} + c^{\varphi^0}, \quad c^{\mathrm{tot}}_a := c^{\mathrm{geo}}_a + c^{\varphi}_a$$

and

$$\begin{aligned}
\kappa c^{\mathrm{geo}} &= \frac{1}{\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right)p^{ab}p^{cd} - \sqrt{q}R^{(3)}, \\
c^{\varphi^0} &= \frac{1}{2}\sqrt{q}\left[\frac{\pi_0^2}{q} + q^{ab}\varphi^0_{,a}\varphi^0_{,b}\right], \\
\kappa c^{\mathrm{geo}}_a &= -2q_{ac}D_b p^{bc}, \\
c^{\varphi}_a &= \pi_0\varphi^0_{,a} + \pi_j\varphi^j_{,a}.
\end{aligned}$$

We need to calculate the Poisson brackets

$$\begin{aligned}
\dot{z} &= \{z, H_{\mathrm{primary}}\} = \{p, H_{\mathrm{primary}}\}, \\
\dot{z}_a &= \{z_a, H_{\mathrm{primary}}\} = \{p_a, H_{\mathrm{primary}}\}, \\
\dot{\Lambda}^{ij} &= \{\Lambda^{ij}, H_{\mathrm{primary}}\} = \{\Pi^{ij}, H_{\mathrm{primary}}\}, \\
\dot{\Phi}_j &= \{\Phi_j, H_{\mathrm{primary}}\} = \{\pi_j - \sqrt{q}M_{jk}\varphi^k_n, H_{\mathrm{primary}}\}.
\end{aligned} \tag{841}$$

D.1.1 Secondary Constraint $\dot{z}$

I. Calculate

$$\begin{aligned}
\dot{z} &= \{z, H_{\mathrm{primary}}\} = \{p, H_{\mathrm{primary}}\} = \int_\chi \mathrm{d}^3x\, \{p, h_{\mathrm{primary}}\} \\
&= \int_\chi \mathrm{d}^3x\, \{p, \nu z + \nu^b z_b + \rho^j\Phi_j + \mu_{ij}\Lambda^{ij} + nc^{\mathrm{tot},0} + n^b c^{\mathrm{tot}}_b + \frac{n}{2}\varphi^j_n\pi_j + \frac{n}{2}\sqrt{q}M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b} + \frac{n}{2}\varphi^j_n\Phi_j\}
\end{aligned} \tag{842}$$

1. $\int_\chi \mathrm{d}^3x\, \{p, \nu z\} = \int_\chi \mathrm{d}^3x\, \nu\{p,p\} = 0$
2. $\int_\chi \mathrm{d}^3x\, \{p, \nu^b z_b\} = \int_\chi \mathrm{d}^3x\, \nu^b\{p, p_b\} = 0$
3. $\int_\chi \mathrm{d}^3x\, \{p, \rho^j\Phi_j\} = \int_\chi \mathrm{d}^3x\, \rho^j\{p, \pi_j - \sqrt{q}M_{jk}\varphi^k_n\} = \int_\chi \mathrm{d}^3x \left(\rho^j\underbrace{\{p,\pi_j\}}_{=0} - \rho^j\sqrt{q}M_{jk}\{p, \tfrac{1}{n}\left(\dot{\varphi}^k - n^a\varphi^k_{,a}\right)\}\right)$
$= -\int_\chi \mathrm{d}^3x\, \rho^j\sqrt{q}M_{jk}\left(\dot{\varphi}^k - n^a\varphi^k_{,a}\right)\{p, \tfrac{1}{n}\} = -\int_\chi \mathrm{d}^3x\, \rho^j\sqrt{q}M_k\tfrac{1}{n}\varphi^k_n\delta^{(3)}(x,y)$
$= -\rho^j\sqrt{q}M_{jk}\tfrac{1}{n}\varphi^k_n$, where we used that $\{p, \tfrac{1}{n}\} = \tfrac{1}{n^2}\delta^{(3)}(x,y)$.

4. $\int\limits_\chi \mathrm{d}^3x\,\{p,\mu_{ij}\Lambda^{ij}\} = \int\limits_\chi \mathrm{d}^3x\,\mu_{ij}\{p,\Pi^{ij}\} = 0$

5. $\int\limits_\chi \mathrm{d}^3x\,\{p,nc^{\mathrm{tot},0}\} = \int\limits_\chi \mathrm{d}^3x\,\left(c^{\mathrm{geo}}+c^{\varphi^0}\right)\underbrace{\{p,n\}}_{-\delta^{(3)}(x,y)} = -c^{\mathrm{tot},0}$

6. $\int\limits_\chi \mathrm{d}^3x\,\{p,n^b c_b^{\mathrm{tot}}\} = 0$

7. $\int\limits_\chi \mathrm{d}^3x\,\{p,\frac{n}{2}\varphi_n^j\pi_j\} = \int\limits_\chi \mathrm{d}^3x\,\{p,\frac{1}{2}\left(\dot{\varphi}^j - n^a\varphi^j_{,a}\right)\pi_j\} = 0$

8. $\int\limits_\chi \mathrm{d}^3x\,\{p,\frac{n}{2}\sqrt{q}M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b}\} = \int\limits_\chi \mathrm{d}^3x\,\frac{1}{2}\sqrt{q}M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b}\underbrace{\{p,n\}}_{-\delta^{(3)}(x,y)} = -\frac{1}{2}\sqrt{q}M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b}$

9. $\int\limits_\chi \mathrm{d}^3x\,\{p,\frac{n}{2}\varphi_n^j\Phi_j\} = \int\limits_\chi \mathrm{d}^3x\left(\{p,\frac{n}{2}\varphi_n^j\}\Phi_j + \varphi_n^j\{p,\frac{n}{2}\Phi_j\}\right)$
$= \int\limits_\chi \mathrm{d}^3x\,\varphi_n^j\{p,\frac{n}{2}\left(\pi_j - \sqrt{q}M_{jk}\varphi_n^k\right)\} = -\frac{1}{2}\varphi_n^j\pi_j$

In summary we obtain

$$\begin{aligned}\dot{z} &= \{p,H_{\mathrm{primary}}\} \\ &= -\frac{1}{n}\rho^j\sqrt{q}M_{jk}\varphi_n^k - c^{\mathrm{tot},0} - \frac{1}{2}\sqrt{q}M_{ij}q^{ab}\varphi^i_{,a}\varphi^j_{,b} - \frac{1}{2}\varphi_n^j\pi_j.\end{aligned} \tag{843}$$

D.1.2 Secondary Constraint $\dot{z}_a$

II. Calculate

$$\dot{z}_a = \{z_a,H_{\mathrm{primary}}\} = \{p_a,H_{\mathrm{primary}}\} = \int\limits_\chi \mathrm{d}^3x\,\{p_a,h_{\mathrm{primary}}\} \tag{844}$$

$$= \int\limits_\chi \mathrm{d}^3x\,\{p_a,\nu z + \nu^b z_b + \rho^j\Phi_j + \mu_{ij}\Lambda^{ij} + nc^{\mathrm{tot},0} + n^b c_b^{\mathrm{tot}} + \frac{n}{2}\varphi_n^j\pi_j + \frac{n}{2}\sqrt{q}M_{ij}q^{cd}\varphi^i_{,c}\varphi^j_{,d} + \frac{n}{2}\varphi_n^j\Phi_j\}$$

1. $\int\limits_\chi \mathrm{d}^3x\,\{p_a,\nu z\} = \int_\chi \mathrm{d}^3x\,\nu\{p_a,p\} = 0$

2. $\int\limits_\chi \mathrm{d}^3x\,\{p_a,\nu^b z_b\} = \int_\chi \mathrm{d}^3x\,\nu^b\{p_a,p_b\} = 0$

3. $\int\limits_\chi \mathrm{d}^3x\,\{p_a,\rho^j\Phi_j\} = \int_\chi \mathrm{d}^3x\,\rho^j\{p_a,\pi_k - \sqrt{q}M_{jk}\varphi_n^k\}$
$= \int\limits_\chi \mathrm{d}^3x\left(\rho^j\underbrace{\{p_a,\pi_j\}}_{=0} - \rho^j\sqrt{q}M_{jk}\{p_a,\frac{1}{n}\left(\dot{\varphi}^k - n^b\varphi^k_{,b}\right)\}\right) = \int\limits_\chi \mathrm{d}^3x\left(\rho^j\sqrt{q}M_{jk}\frac{1}{n}\varphi^k_{,b}\underbrace{\{p_a,n^b\}}_{-\delta^b_a\delta^{(3)}(x,y)}\right)$
$= -\int\limits_\chi \mathrm{d}^3x\,\rho^j\sqrt{q}M_{jk}\frac{1}{n}\varphi^k_{,a}\delta^{(3)}(x,y) = -\rho^j\sqrt{q}M_{jk}\frac{1}{n}\varphi^k_{,a}$

4. $\int\limits_\chi \mathrm{d}^3x\,\{p_a,\mu_{ij}\Lambda^{ij}\} = \int\limits_\chi \mathrm{d}^3x\,\mu_{ij}\{p_a,\Pi^{ij}\} = 0$

5. $\int_\chi \mathrm{d}^3x\,\{p_a, nc^{\mathrm{tot},0}\} = \int_\chi \mathrm{d}^3x\,\{p_a, n\left(c^{\mathrm{geo}} + c^{\varphi^0}\right)\} = 0$

6. $\int_\chi \mathrm{d}^3x\,\{p_a, n^b c_b^{\mathrm{tot}}\} = -c_a^{\mathrm{tot}}$

7. $\int_\chi \mathrm{d}^3x\,\{p_a, \frac{n}{2}\varphi_n^j\pi_j\} = \int_\chi \mathrm{d}^3x\,\{p_a, \frac{n}{2}\frac{1}{n}\left(\dot{\varphi}^j - n^b\varphi^j_{,b}\right)\pi_j\}$
$= -\int_\chi \mathrm{d}^3x\,\frac{1}{2}\varphi^j_{,b}\pi_j \underbrace{\{p_a, n^b\}}_{-\delta^b_a\delta^{(3)}(x,y)} = \frac{1}{2}\varphi^j_{,a}\pi_j$

8. $\int_\chi \mathrm{d}^3x\,\{p_a, \frac{n}{2}\sqrt{q}M_{ij}q^{cd}\varphi^i_{,c}\varphi^j_{,d}\} = 0$

9. $\int_\chi \mathrm{d}^3x\,\{p_a, \frac{n}{2}\varphi_n^j\Phi_j\} = \int_\chi \mathrm{d}^3x\left(\{p_a, \frac{n}{2}\varphi_n^j\}\Phi_j + \varphi_n^j\{p_a, \frac{n}{2}\Phi_j\}\right)$
$= \int_\chi \mathrm{d}^3x\left(\frac{n}{2}\{p_a, \varphi_n^j\}\Phi_j + \frac{n}{2}\varphi_n^j\{p_a, \left(\pi_j - \sqrt{q}M_{jk}\varphi_n^k\right)\}\right)$
$= \int_\chi \mathrm{d}^3x\left(\frac{1}{2}\varphi^j_{,a}\Phi_j\delta^{(3)}(x,y) - \frac{n}{2}\varphi_n^j\sqrt{q}M_{jk}\{p_a, \varphi_n^k\}\right)$
$= \int_\chi \mathrm{d}^3x\left(\frac{1}{2}\varphi^j_{,a}\Phi_j\delta^{(3)}(x,y) - \frac{1}{2}\varphi_n^j\sqrt{q}M_{jk}\varphi^k_{,a}\delta^{(3)}(x,y)\right)$
$= \frac{1}{2}\varphi^j_{,a}\Phi_j - \frac{1}{2}\varphi_n^j\sqrt{q}M_{jk}\varphi^k_{,a}$, where we used that $M_{jk} = M_{kj}$ and
$\{p_a, \varphi_n^j\} = \{p_a, \frac{1}{n}\left(\dot{\varphi}^j - n^b\varphi^j_{,b}\right)\} = -\frac{1}{n}\varphi^j_{,b}\underbrace{\{p_a, n^b\}}_{-\delta^b_a\delta^{(3)}(x,y)} = \frac{1}{n}\varphi^j_{,a}\delta^{(3)}(x,y)$

In summary we obtain

$$\dot{z}_a = \{p_a, H_{\mathrm{primary}}\} = -\rho^j\sqrt{q}M_{jk}\frac{1}{n}\varphi^k_{,a} - c_a^{\mathrm{tot}} + \frac{1}{2}\varphi^j_{,a}\pi_j + \frac{1}{2}\varphi^j_{,a}\Phi_j - \frac{1}{2}\varphi_n^j\sqrt{q}M_{jk}\varphi^k_{,a}. \tag{845}$$

D.1.3 Secondary Constraint $\dot{\Lambda}^{ij}$

III. Calculate

$$\dot{\Lambda}^{ij} = \{\Lambda^{ij}, H_{\mathrm{primary}}\} = \{\Pi^{ij}, H_{\mathrm{primary}}\} = \int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, h_{\mathrm{primary}}\} \tag{846}$$

$$= \int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, \nu z + \nu^b z_b + \rho^k\Phi_k + \mu_{k\ell}\Lambda^{k\ell} + nc^{\mathrm{tot},0} + n^b c_b^{\mathrm{tot}} + \frac{n}{2}\varphi_n^k\pi_k + \frac{n}{2}\sqrt{q}M_{k\ell}q^{ab}\varphi^k_{,a}\varphi^\ell_{,b} + \frac{n}{2}\varphi_n^k\Phi_k\}$$

1. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, \nu z\} = \int_\chi \mathrm{d}^3x\,\nu\{\Pi^{ij}, p\} = 0$

2. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, \nu^b z_b\} = \int_\chi \mathrm{d}^3x\,\nu^b\{\Pi^{ij}, p_b\} = 0$

3. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, \rho^k\Phi_k\} = \int_\chi \mathrm{d}^3x\,\rho^k\{\Pi^{ij}, \pi_k - \sqrt{q}M_{k\ell}\varphi_n^\ell\}$
$= \int_\chi \mathrm{d}^3x\left(\rho^k\underbrace{\{\Pi^{ij}, \pi_k\}}_{=0} - \rho^k\sqrt{q}\varphi_n^\ell\underbrace{\{\Pi^{ij}, M_{k\ell}\}}_{-\delta^i_{(k}\delta^j_{\ell)}\delta^{(3)}(x,y)}\right) = \int_\chi \mathrm{d}^3x\,\rho^k\sqrt{q}\varphi_n^\ell\delta^i_k\delta^j_\ell\delta^{(3)}(x,y)$
$= \int_\chi \mathrm{d}^3x\,\rho^i\sqrt{q}\varphi_n^j\delta^{(3)}(x,y) = \rho^i\sqrt{q}\varphi_n^j$, where we used that $M_{k\ell} = M_{\ell k}$.

4. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, \mu_{k\ell}\Lambda^{k\ell}\} = \int_\chi \mathrm{d}^3x\,\mu_{k\ell}\{\Pi^{ij}, \Pi^{k\ell}\} = 0$

5. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, nc^{\mathrm{tot},0}\} = \int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, n\left(c^{\mathrm{geo}} + c^{\varphi^0}\right)\} = 0$

6. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, n^b c_b^{\mathrm{tot}}\} = \int_\chi \mathrm{d}^3x\,n^b\{\Pi^{ij}, c_b^{\mathrm{tot}}\} = 0$

7. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, \frac{n}{2}\varphi_n^k\pi_k\} = 0$

8. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, \frac{n}{2}\sqrt{q}M_{k\ell}q^{ab}\varphi^k_{,a}\varphi^\ell_{,b}\} = \int_\chi \mathrm{d}^3x\,\frac{n}{2}\sqrt{q}q^{ab}\varphi^k_{,a}\varphi^\ell_{,b}\,\underbrace{\{\Pi^{ij}, M_{k\ell}\}}_{-\delta^i_{(k}\delta^j_{\ell)}\delta^{(3)}(x,y)}$
$= -\int_\chi \mathrm{d}^3x\,\frac{n}{2}\sqrt{q}q^{ab}\varphi^i_{,a}\varphi^j_{,b}\delta^{(3)}(x,y) = -\frac{n}{2}\sqrt{q}q^{ab}\varphi^i_{,a}\varphi^j_{,b}$, where we used that $M_{k\ell} = M_{\ell k}$.

9. $\int_\chi \mathrm{d}^3x\,\{\Pi^{ij}, \frac{n}{2}\varphi_n^k\Phi_k\} = \int_\chi \mathrm{d}^3x\,\frac{n}{2}\varphi_n^k\{\Pi^{ij}, \pi_k - \sqrt{q}M_{k\ell}\varphi_n^\ell\}$
$= \int_\chi \mathrm{d}^3x\left(\frac{n}{2}\varphi_n^k\underbrace{\{\Pi^{ij}, \pi_k\}}_{=0} - \sqrt{q}\frac{n}{2}\varphi_n^k\varphi_n^\ell\underbrace{\{\Pi^{ij}, M_{k\ell}\}}_{-\delta^i_{(k}\delta^j_{\ell)}\delta^{(3)}(x,y)}\right) = \int_\chi \mathrm{d}^3x\,\sqrt{q}\frac{n}{2}\varphi_n^k\varphi_n^\ell\delta^i_k\delta^j_\ell\delta^{(3)}(x,y)$
$= \int_\chi \mathrm{d}^3x\,\sqrt{q}\frac{n}{2}\varphi_n^i\varphi_n^j\delta^{(3)}(x,y) = \sqrt{q}\frac{n}{2}\varphi_n^i\varphi_n^j$, where we used that $M_{k\ell} = M_{\ell k}$.

In summary we obtain

$$\dot{\Lambda}^{ij} = \{\Pi^{ij}, H_{\mathrm{primary}}\} = \rho^i\sqrt{q}\varphi_n^j + \frac{n}{2}\sqrt{q}\left(\varphi_n^i\varphi_n^j - q^{ab}\varphi^i_{,a}\varphi^j_{,b}\right). \tag{847}$$

D.1.4 Secondary Constraint $\dot{\Phi}_i$

IV. Calculate

$$\dot{\Phi}_j = \{\Phi_j(x), H_{\mathrm{primary}}(y)\} = \int_\chi \mathrm{d}^3y\,\{\Phi_j(x), h_{\mathrm{primary}}(y)\} \tag{848}$$
$$= \int_\chi \mathrm{d}^3y\,\{\Phi_j(x), \left[\nu z + \nu^b z_b + \rho^k\Phi_k + \mu_{k\ell}\Lambda^{k\ell} + nc^{\mathrm{tot},0} + n^b c_b^{\mathrm{tot}} + \frac{n}{2}\varphi_n^k\pi_k + \frac{n}{2}\sqrt{q}M_{k\ell}q^{ab}\varphi^k_{,a}\varphi^\ell_{,b} + \frac{n}{2}\varphi_n^k\Phi_k\right](y)\}.$$

1. $\int_\chi \mathrm{d}^3y\,\{\Phi_j, \nu z\} = \int_\chi \mathrm{d}^3y\,\{\pi_j - \sqrt{q}M_{ji}\varphi_n^i, \nu z\}$
$= \int_\chi \mathrm{d}^3y\,\nu\{\pi_j - \sqrt{q}M_{ji}\varphi_n^i, p\} = \int_\chi \mathrm{d}^3y\left(\nu\underbrace{\{\pi_j, p\}}_{=0} - \nu\sqrt{q}M_{ji}\{\frac{1}{n}\left(\dot{\varphi}^i - n^b\varphi^i_{,b}\right), p\}\right)$
$= -\int_\chi \mathrm{d}^3y\,\nu\sqrt{q}M_{ji}\left(\dot{\varphi}^i - n^b\varphi^i_{,b}\right)\{\frac{1}{n}, p\} = \int_\chi \mathrm{d}^3y\,\nu\sqrt{q}M_{ji}\frac{1}{n}\varphi_n^i\delta^{(3)}(x,y)$
$= \nu\sqrt{q}M_{ji}\frac{1}{n}\varphi_n^i$, where we used that $\{\frac{1}{n}, p\} = -\frac{1}{n^2}\delta^{(3)}(x,y)$.

2. $\int_\chi \mathrm{d}^3y\,\{\Phi_j, \nu^b z_b\} = \int_\chi \mathrm{d}^3y\,\{\pi_j - \sqrt{q}M_{ji}\varphi_n^i, \nu^b z_b\}$
$= \int_\chi \mathrm{d}^3y\,\nu^b\{\pi_j - \sqrt{q}M_{ji}\varphi_n^i, p_b\} = \int_\chi \mathrm{d}^3y\left(\nu^b\underbrace{\{\pi_j, p_b\}}_{=0} - \nu^b\sqrt{q}M_{ji}\{\frac{1}{n}\left(\dot{\varphi}^i - n^a\varphi^i_{,a}\right), p_b\}\right)$

$$= \int_\chi \mathrm{d}^3y\, \nu^b \sqrt{q} M_{ji} \tfrac{1}{n} \varphi^i_{,a} \underbrace{\{n^a, p_b\}}_{\delta^a_b \delta^{(3)}(x,y)} = \int_\chi \mathrm{d}^3y\, \nu^b \sqrt{q} M_{ji} \tfrac{1}{n} \varphi^i_{,b} \delta^{(3)}(x,y)$$
$$= \nu^b \sqrt{q} M_{ji} \tfrac{1}{n} \varphi^i_{,b}$$

3. $\int_\chi \mathrm{d}^3y\, \{\Phi_j, \rho^k \Phi_k\} = \int_\chi \mathrm{d}^3y\, \rho^k \{\Phi_j, \Phi_k\}$
$$= \int_\chi \mathrm{d}^3y\, \rho^k \{\left[\pi_j - \sqrt{q} M_{ji} \varphi^i_n\right](x), [\Phi_k](y)\}$$
$$= \int_\chi \mathrm{d}^3y\, \rho^k(y) \{\left[\pi_j - \sqrt{q} M_{ji} \varphi^i_n\right](x), \left[\pi_k - \sqrt{q} M_{k\ell} \varphi^\ell_n\right](y)\}$$
$$= \int_\chi \mathrm{d}^3y \Bigg(\rho^k(y) \underbrace{\{\pi_j(x), \pi_k(y)\}}_{=0} - \rho^k(y) \{\left[\sqrt{q} M_{ji} \varphi^i_n\right](x), \pi_k(y)\}$$
$$- \rho^k(y) \{\pi_j(x), \left[\sqrt{q} M_{k\ell} \varphi^\ell_n\right](y)\} + \rho^k(y) \underbrace{\{\left[\sqrt{q} M_{ji} \varphi^i_n\right](x), \left[\sqrt{q} M_{k\ell} \varphi^\ell_n\right](y)\}}_{=0} \Bigg)$$
$$= \int_\chi \mathrm{d}^3y\, \left(-\rho^k(y) \left[\sqrt{q} M_{ji}\right](x) \{\varphi^i_n(x), \pi_k(y)\} - \left[\rho^k \sqrt{q} M_{k\ell}\right](y) \{\pi_j(x), \varphi^\ell_n(y)\} \right)$$
$$= \int_\chi \mathrm{d}^3y\, \left(-\rho^k(y) \left[\tfrac{1}{n} \sqrt{q} M_{ji}\right](x) \{\left(\dot\varphi^i - n^a \varphi^i_{,a}\right)(x), \pi_k(y)\} \right.$$
$$\left. - \left[\rho^k \tfrac{1}{n} \sqrt{q} M_{k\ell}\right](y) \{\pi_j(x), \left(\dot\varphi^\ell - n^b \varphi^\ell_{,b}\right)(y)\} \right)$$
$$= \int_\chi \mathrm{d}^3y \Bigg(- \rho^k(y) \left[\tfrac{1}{n} \sqrt{q} M_{ji}\right](x) \left(\partial_t \delta^{(3)}(x,y) - n^a(x) \tfrac{\partial}{\partial x^a} \delta^{(3)}(x,y)\right) \delta^i_k$$
$$+ \left[\rho^k \tfrac{1}{n} \sqrt{q} M_{k\ell}\right](y) \left(\partial_t \delta^{(3)}(x,y) - n^b(y) \tfrac{\partial}{\partial y^b} \delta^{(3)}(x,y)\right) \delta^\ell_j \Bigg)$$
$$= \int_\chi \mathrm{d}^3y \left(\rho^k(y) \left[\tfrac{1}{n} \sqrt{q} n^a M_{jk}\right](x) \tfrac{\partial}{\partial x^a} \delta^{(3)}(x,y) - \left[\rho^k \tfrac{1}{n} n^b \sqrt{q} M_{jk}\right](y) \tfrac{\partial}{\partial y^b} \delta^{(3)}(x,y) \right)$$
$$= \int_\chi \mathrm{d}^3y \left(- \rho^k(y) \left[\tfrac{1}{n} \sqrt{q} n^a M_{jk}\right](x) \tfrac{\partial}{\partial y^a} \delta^{(3)}(x,y) - \left[\rho^k \tfrac{1}{n} \sqrt{q} n^b M_{jk}\right](y) \tfrac{\partial}{\partial y^b} \delta^{(3)}(x,y) \right)$$
$$= \rho^k_{,a} \left[\tfrac{1}{n} n^a \sqrt{q} M_{jk}\right] + \left[\rho^k \tfrac{1}{n} n^a \sqrt{q} M_{jk}\right]_{,a} = \rho^k \left[\tfrac{1}{n} n^a \sqrt{q} M_{jk}\right]_{,a} + 2\rho^k_{,a} \left[\tfrac{1}{n} n^a \sqrt{q} M_{jk}\right]$$

4. $\int_\chi \mathrm{d}^3y\, \{\Phi_j, \mu_{k\ell} \Lambda^{k\ell}\} = \int_\chi \mathrm{d}^3y\, \mu_{k\ell} \{\pi_j - \sqrt{q} M_{ji} \varphi^i_n, \Pi^{k\ell}\}$
$$= \int_\chi \mathrm{d}^3y \left(\mu_{k\ell} \underbrace{\{\pi_j, \Pi^{k\ell}\}}_{=0} - \mu_{k\ell} \sqrt{q} \varphi^i_n \{M_{ji}, \Pi^{k\ell}\} \right) = - \int_\chi \mathrm{d}^3y\, \mu_{k\ell} \sqrt{q} \varphi^i_n \delta^k_j \delta^\ell_i \delta^{(3)}(x,y)$$
$$= - \int_\chi \mathrm{d}^3y\, \mu_{ji} \sqrt{q} \varphi^i_n \delta^{(3)}(x,y) = -\mu_{ji} \sqrt{q} \varphi^i_n$$

5. $\int_\chi \mathrm{d}^3y\, \{\Phi_j, nc^{\mathrm{tot},0}\} = \int_\chi \mathrm{d}^3y\, \{\pi_j - \sqrt{q} M_{ji} \varphi^i_n, nc^{\mathrm{tot},0}\}$
$$= \int_\chi \mathrm{d}^3y\, \left(\{\pi_j, nc^{\mathrm{tot},0}\} - \{\sqrt{q} M_{ji} \varphi^i_n, nc^{\mathrm{tot},0}\} \right)$$
$$= \int_\chi \mathrm{d}^3y \left(\underbrace{\{\pi_j, nc^{\mathrm{geo}}\}}_{=0} + \underbrace{\{\pi_j, nc^{\varphi^0}\}}_{=0} - \{\sqrt{q} M_{ji} \varphi^i_n, nc^{\mathrm{geo}}\} - \underbrace{\{\sqrt{q} M_{ji} \varphi^i_n, nc^{\varphi^0}\}}_{=0} \right)$$
$$= - \int_\chi \mathrm{d}^3y\, \{\left[\sqrt{q} M_{ji} \varphi^i_n\right](x), n(y) c^{\mathrm{geo}}(y)\}$$
$$= - \int_\chi \mathrm{d}^3y\, \left[M_{ji} \varphi^i_n\right](x) \{\sqrt{q}(x), n(y) c^{\mathrm{geo}}(y)\}$$

$$= -\int_\chi \mathrm{d}^3y \, \left(\left[M_{ji}\varphi^i_n\right](x) \tfrac{n(y)}{\kappa\sqrt{q}(y)} \left[q_{ac}q_{bd} - \tfrac{1}{2}q_{ab}q_{cd}\right](y) \left(p^{ab}(y)\{\sqrt{q}(x), p^{cd}(y)\} + \{\sqrt{q}(x), p^{ab}(y)\}p^{cd}(y)\right)\right)$$
$$= -\int_\chi \mathrm{d}^3y \, \left(\left[M_{ji}\varphi^i_n\right](x) \tfrac{n(y)}{\kappa\sqrt{q}(y)} \left[q_{ac}q_{bd} - \tfrac{1}{2}q_{ab}q_{cd}\right](y) \tfrac{\kappa}{2}\sqrt{q}(x) \left(p^{ab}(y)q^{cd}(x) + q^{ab}(x)p^{cd}(y)\right)\delta^{(3)}(x,y)\right)$$
$$= -\tfrac{n}{2}M_{ji}\varphi^i_n \left(q_{ab}p^{ab} - \tfrac{1}{2}q_{ab}p^{ab}\underbrace{\delta^c_c}_{=3} + q_{cd}p^{cd} - \tfrac{1}{2}q_{cd}p^{cd}\underbrace{\delta^a_a}_{=3}\right)$$
$= \frac{n}{2}M_{ji}\varphi^i_n q_{ab}p^{ab}$, where we used that $q^{ab} = q^{ba}$ and $M_{ji} = M_{ij}$ are symmetric.

For the calculation under 5. we needed to calculate the Poisson bracket of $\sqrt{q}$ and p^{ab}. We know that $\delta q = qq^{ab}\delta q_{ab}$, see for example [9]. From this follows

$$\delta\sqrt{q} = \frac{1}{2}\frac{1}{\sqrt{q}}\delta q = \frac{1}{2}\frac{1}{\sqrt{q}}qq^{ab}\delta q_{ab} = \frac{1}{2}\sqrt{q}q^{ab}\delta q_{ab}. \tag{849}$$

For the Poisson bracket of $\sqrt{q}$ and p^{ab} this means

$$\begin{aligned}\{\sqrt{q}, p^{ab}\} &= \frac{1}{2}\sqrt{q}q^{cd}\{q_{cd}, p^{ab}\} = \frac{1}{2}\sqrt{q}q^{cd}\kappa\delta^a_{(c}\delta^b_{d)}\delta^{(3)}(x,y) = \frac{\kappa}{2}\sqrt{q}q^{cd}\frac{1}{2}\left(\delta^a_c\delta^b_d + \delta^a_d\delta^b_c\right)\delta^{(3)}(x,y) \\ &= \frac{\kappa}{2}\sqrt{q}\frac{1}{2}\left(q^{ab} + q^{ba}\right)\delta^{(3)}(x,y) = \frac{\kappa}{2}\sqrt{q}q^{ab}\delta^{(3)}(x,y),\end{aligned} \tag{850}$$

since $q^{ab} = q^{ba}$ is symmetric.

6. $\int_\chi \mathrm{d}^3y \, \{\Phi_j, n^b c^{\mathrm{tot}}_b\} = \int_\chi \mathrm{d}^3y \, \{\pi_j - \sqrt{q}M_{ji}\varphi^i_n, n^a c^{\mathrm{tot}}_a\} = \int_\chi \mathrm{d}^3y \, \{\pi_j - \sqrt{q}M_{ji}\varphi^i_n, n^a \left(c^{\mathrm{geo}}_a + c^\varphi_a\right)\}$

$$= \int_\chi \mathrm{d}^3y \left(\underbrace{\{\pi_i, n^a c^{\mathrm{geo}}_a + c^\varphi_a\}}_{=0} - \{\sqrt{q}M_{ji}\varphi^i_n, n^a c^{\mathrm{geo}}_a\} - \underbrace{\{\sqrt{q}M_{ji}\varphi^i_n, n^a c^\varphi_a\}}_{=0}\right)$$
$$= -\int_\chi \mathrm{d}^3y \, \{\left[\sqrt{q}M_{ij}\varphi^j_n\right](x), [n^a c^{\mathrm{geo}}_a](y)\}$$
$$= M_{ji}\varphi^i_n \left(-\sqrt{q}q^{bc}\left[n^a q_{ac}\right]_{,b} + \sqrt{q}q^{fc}n^a q_{ac}\Gamma^c_{fb} + \sqrt{q}q^{bf}n^a q_{ac}\Gamma^b_{fb}\right)$$
$$= M_{ji}\varphi^i_n \left(-\sqrt{q}q^{bc}n^a_{,b}q_{ac} - \sqrt{q}q^{bc}n^a q_{ac,b} + \sqrt{q}q^{fc}n^a q_{ac}\Gamma^c_{fb} + \sqrt{q}q^{bf}n^a q_{ac}\Gamma^b_{fb}\right)$$
$$= M_{ji}\varphi^i_n \left(-\sqrt{q}n^a_{,b}q_{ac}q^{bc} + \sqrt{q}n^a q_{ac}q^{bc}_{,b} + \sqrt{q}n^a q_{ac}q^{fc}\Gamma^c_{fb} + \sqrt{q}n^a q_{ac}q^{bf}\Gamma^b_{fb}\right)$$
$$= -\sqrt{q}M_{ji}\varphi^i_n n^a_{,b}\delta^b_a + \sqrt{q}M_{ji}\varphi^i_n n^a q_{ac}D_b q^{bc}$$
$$= \sqrt{q}M_{ji}\varphi^i_n\left(-n^a_{,a} + n^a q_{ac}D_b q^{bc}\right),$$

where we used that

$$\{\sqrt{q}(x), n^a c_a^{\mathrm{geo}}(y)\} = \{\sqrt{q}(x), \left[-\frac{2}{\kappa} n^a q_{ac}\, D_b p^{bc}\right](y)\} \tag{851}$$
$$= -\frac{2}{\kappa}\left[n^a q_{ac}\right](y)\{\sqrt{q}(x), D_b p^{bc}(y)\}$$
$$= -\frac{2}{\kappa}\left[n^a q_{ac}\right](y)\{\sqrt{q}(x), \partial_b p^{bc}(y) + \Gamma^b_{fb} p^{fc}(y) + \Gamma^c_{fb} p^{bf}(y)\}$$
$$= -\frac{2}{\kappa}\left[n^a q_{ac}\right](y)\{\sqrt{q}(x), \partial_b p^{bc}(y)\} - \frac{2}{\kappa}\left[n^a q_{ac}\Gamma^b_{fb}\right](y)\{\sqrt{q}(x), p^{fc}(y)\}$$
$$- \frac{2}{\kappa}\left[n^a q_{ac}\Gamma^c_{fb}\right](y)\{\sqrt{q}(x), p^{bf}(y)\}$$
$$= -\frac{2}{\kappa}\left[\frac{1}{2}\sqrt{q}q^{gh}\right](x)\left[n^a q_{ac}\right](y)\{q_{gh}(x), \partial_b p^{bc}(y)\} - \frac{2}{\kappa}\left[\frac{1}{2}\sqrt{q}q^{gh}\right](x)\left[n^a q_{ac}\Gamma^c_{fb}\right](y)\{q_{gh}(x), p^{fc}(y)\}$$
$$- \frac{2}{\kappa}\left[\frac{1}{2}\sqrt{q}q^{gh}\right](x)\left[n^a q_{ac}\Gamma^b_{fb}\right](y)\{q_{gh}(x), p^{bf}(y)\}$$
$$= -\frac{1}{\kappa}\left[\sqrt{q}q^{gh}\right](x)\left[n^a q_{ac}\right](y)\,\kappa\delta^b_{(g}\delta^c_{h)}\frac{\partial}{\partial y^b}\delta^{(3)}(x,y) - \frac{1}{\kappa}\left[\sqrt{q}q^{gh}\right](x)\left[n^a q_{ac}\Gamma^c_{fb}\right](y)\,\kappa\delta^f_{(g}\delta^c_{h)}\delta^{(3)}(x,y)$$
$$- \frac{1}{\kappa}\left[\sqrt{q}q^{gh}\right](x)\left[n^a q_{ac}\Gamma^b_{fb}\right](y)\,\kappa\delta^b_{(g}\delta^f_{h)}\delta^{(3)}(x,y)$$
$$= -\left[\sqrt{q}q^{bc}\right](x)\left[n^a q_{ac}\right](y)\frac{\partial}{\partial y^b}\delta^{(3)}(x,y) - \left[\sqrt{q}q^{fc}\right](x)\left[n^a q_{ac}\Gamma^c_{fb}\right](y)\,\delta^{(3)}(x,y)$$
$$- \left[\sqrt{q}q^{bf}\right](x)\left[n^a q_{ac}\Gamma^b_{fb}\right](y)\,\delta^{(3)}(x,y).$$

7. $\int_\chi \mathrm{d}^3y\,\{\Phi_j, \frac{n}{2}\varphi^k_n\pi_k\} = \int_\chi \mathrm{d}^3y\,\{\pi_j - \sqrt{q}M_{ji}\varphi^i_n, \frac{n}{2}\varphi^k_n\pi_k\}$
$= \int_\chi \mathrm{d}^3y\left(\left[\frac{n}{2}\pi_k\right](y)\{\pi_j(x), \varphi^k_n(y)\} - \left[\frac{n}{2}\varphi^k_n\right](y)\left[\sqrt{q}M_{ji}\right](x)\{\varphi^i_n(x), \pi_k(y)\}\right)$
$= \int_\chi \mathrm{d}^3y\left(-\left[\frac{n}{2}\pi_k\right](y)\{\varphi^k_n(y), \pi_j(x)\} - \left[\frac{n}{2}\varphi^k_n\right](y)\left[\sqrt{q}M_{ji}\right](x)\{\varphi^i_n(x), \pi_k(y)\}\right)$
$= \int_\chi \mathrm{d}^3y\left(-\left[\frac{1}{2}\pi_k(y)\right]\delta^k_j\left(\frac{\partial}{\partial t}\delta^{(3)}(x,y) - n^a(y)\frac{\partial}{\partial y^a}\delta^{(3)}(x,y)\right)\right.$
$\left.- \left[\frac{n}{2}\varphi^k_n\right](y)\left[\frac{1}{n}\sqrt{q}M_{ji}\right](x)\delta^i_k\left(\frac{\partial}{\partial t}\delta^{(3)}(x,y) - n^a(x)\frac{\partial}{\partial x^a}\delta^{(3)}(x,y)\right)\right)$
$= \int_\chi \mathrm{d}^3y\left(\left[\frac{1}{2}n^a\pi_j\right](y)\frac{\partial}{\partial y^a}\delta^{(3)}(x,y) + \left[\frac{n}{2}\varphi^k_n\right](y)\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right](x)\frac{\partial}{\partial x^a}\delta^{(3)}(x,y)\right)$
$= \int_\chi \mathrm{d}^3y\left(\left[\frac{1}{2}n^a\pi_j\right](y)\frac{\partial}{\partial y^a}\delta^{(3)}(x,y) - \left[\frac{n}{2}\varphi^k_n\right](y)\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right](x)\frac{\partial}{\partial y^a}\delta^{(3)}(x,y)\right)$
$= \left[\frac{1}{2}n^a\pi_j\right]_{,a} - \left[\frac{n}{2}\varphi^k_n\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]$

8. $\int_\chi \mathrm{d}^3y\,\{\Phi_j, \frac{n}{2}\sqrt{q}M_{k\ell}q^{ab}\varphi^k_{,a}\varphi^\ell_{,b}\} = \int_\chi \mathrm{d}^3y\,\{\pi_j - \sqrt{q}M_{ji}\varphi^i_n, \frac{n}{2}\sqrt{q}M_{k\ell}q^{ab}\varphi^k_{,a}\varphi^\ell_{,b}\}$
$= \int_\chi \mathrm{d}^3y\,\left[\frac{n}{2}\sqrt{q}M_{k\ell}q^{ab}\right](y)\{\pi_j(x), \left(\varphi^k_{,a}\varphi^\ell_{,b}\right)(y)\} - \int_\chi \mathrm{d}^3y\,\underbrace{\{\sqrt{q}M_{ji}\varphi^i_n, \frac{n}{2}\sqrt{q}M_{k\ell}q^{ab}\varphi^k_{,a}\varphi^\ell_{,b}\}}_{=0}$
$= \int_\chi \mathrm{d}^3y\,\left[n\sqrt{q}q^{ab}M_{k\ell}\varphi^k_{,a}\right](y)\{\pi_j(x), \varphi^\ell_{,b}(y)\} = -\int_\chi \mathrm{d}^3y\,\left[n\sqrt{q}q^{ab}M_{k\ell}\varphi^k_{,a}\right](y)\delta^\ell_j\frac{\partial}{\partial y^b}\delta^{(3)}(x,y)$
$= \left[n\sqrt{q}q^{ab}M_{kj}\varphi^k_{,a}\right]_{,b}$, where we used that $q^{ab} = q^{ba}$ is symmetric.

9. $\int_\chi \mathrm{d}^3y\,\{\Phi_j, \frac{n}{2}\varphi^k_n\Phi_k\} = \int_\chi \mathrm{d}^3y\,\left(\left[\frac{n}{2}\varphi^k_n\right](y)\{\Phi_j(x), \Phi_k(y)\} + \left[\frac{n}{2}\Phi_k\right](y)\{\Phi_j(x), \varphi^k_n(y)\}\right)$

$= \left[\frac{n}{2}\varphi_n^k\right]\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + 2\left[\frac{n}{2}\varphi_n^k\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] + \int_\chi d^3y\ \left[\frac{n}{2}\Phi_k\right](y)\{\left[\pi_j - \sqrt{q}M_{ji}\varphi_n^i\right](x), \varphi_n^k(y)\}$
$= \left[\frac{n}{2}\varphi_n^k\right]\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + 2\left[\frac{n}{2}\varphi_n^k\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] + \int_\chi d^3y\ \left[\frac{n}{2}\Phi_j n^a\right](y)\frac{\partial}{\partial y^a}\delta^{(3)}(x,y)$
$= \left[\frac{n}{2}\varphi_n^k\right]\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + 2\left[\frac{n}{2}\varphi_n^k\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] - \left[\frac{n}{2}\Phi_j n^a\right]_{,a}$, where we used the results from the calculation in 3. above.

In summary we obtain

$$\begin{aligned}
\dot{\Phi}_j = {} & \nu\sqrt{q}M_{ji}\frac{1}{n}\varphi_n^i + \nu^b\sqrt{q}M_{ji}\frac{1}{n}\varphi_{,b}^i + \rho^k\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + 2\rho_{,a}^k\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] \\
& - \mu_{ji}\sqrt{q}\varphi_n^i + \frac{n}{2}M_{ji}\varphi_n^i q_{ab}p^{ab} + \sqrt{q}M_{ji}\varphi_n^i\left(-n_{,a}^a + n^a q_{ac}D_b q^{bc}\right) \\
& + \left[\frac{1}{2}n^a\pi_j\right]_{,a} - \left[\frac{n}{2}\varphi_n^k\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] + \left[n\sqrt{q}q^{ab}M_{jk}\varphi_{,a}^k\right]_{,b} \\
& + \left[\frac{n}{2}\varphi_n^k\right]\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + 2\left[\frac{n}{2}\varphi_n^k\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] - \left[\frac{n}{2}\Phi_j n^a\right]_{,a}.
\end{aligned} \tag{852}$$

D.2 Summary

We summarize:

$$\begin{aligned}
\dot{z} &= -\frac{1}{n}\rho^k\sqrt{q}M_{k\ell}\varphi_n^\ell - c^{\text{tot},0} - \frac{1}{2}\sqrt{q}M_{ij}q^{ab}\varphi_{,a}^i\varphi_{,b}^j - \frac{1}{2}\varphi_n^j\pi_j, \\
\dot{z}_a &= -\rho^k\sqrt{q}M_{k\ell}\frac{1}{n}\varphi_{,a}^\ell - c_a^{\text{tot}} + \frac{1}{2}\varphi_{,a}^j\pi_j + \frac{1}{2}\varphi_{,a}^j\Phi_j - \frac{1}{2}\varphi_n^j\sqrt{q}M_{j\ell}\varphi_{,a}^\ell, \\
\dot{\Lambda}^{ij} &= \rho^i\sqrt{q}\varphi_n^j + \frac{n}{2}\sqrt{q}\left(\varphi_n^i\varphi_n^j - q^{ab}\varphi_{,a}^i\varphi_{,b}^j\right), \\
\dot{\Phi}_j &= \nu\sqrt{q}M_{ji}\frac{1}{n}\varphi_n^i + \nu^b\sqrt{q}M_{ji}\frac{1}{n}\varphi_{,b}^i + \rho^k\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + 2\rho_{,a}^k\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] \\
& \quad - \mu_{ji}\sqrt{q}\varphi_n^i + \frac{n}{2}M_{ji}\varphi_n^i q_{ab}p^{ab} + \sqrt{q}M_{ji}\varphi_n^i\left(-n_{,a}^a + n^a q_{ac}D_b q^{bc}\right) \\
& \quad + \left[\frac{1}{2}n^a\pi_j\right]_{,a} + \left[n\sqrt{q}q^{ab}M_{jk}\varphi_{,a}^k\right]_{,b} \\
& \quad + \left[\frac{n}{2}\varphi_n^k\right]\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right]_{,a} + \left[\frac{n}{2}\varphi_n^k\right]_{,a}\left[\frac{1}{n}n^a\sqrt{q}M_{jk}\right] - \left[\frac{n}{2}\Phi_j n^a\right]_{,a}.
\end{aligned} \tag{853}$$

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Large parts of this section have been published in [130].

E.1 Constraint Stability Analysis

In the following we need to perform the constraint analysis in order to check whether the primary constraints are stable under time evolution with respect to $H_{primary}$ or not. The non-vanishing

Poisson brackets on the phase space are given by

$$\begin{aligned}
\{q_{cd}(x), p^{ab}(y)\} &= \kappa\delta^a_{(c}\delta^b_{d)}\delta^{(3)}(x,y), \\
\{n(x), p(y)\} &= \delta^{(3)}(x,y), \\
\{n^a(x), p_b(y)\} &= \delta^a_b\delta^{(3)}(x,y), \\
\{\varphi^0(x), \pi_0(y)\} &= \delta^{(3)}(x,y), \\
\{\varphi^j(x), \pi_k(y)\} &= \delta^j_k\delta^{(3)}(x,y), \\
\{M_{jj}(x), \Pi^{kk}(y)\} &= \delta^k_j\delta^{(3)}(x,y).
\end{aligned} \tag{854}$$

We need to calculate the Poisson brackets or respectively secondary constrainst

$$\begin{aligned}
&\dot{z} = \{z, H_{\text{primary}}\} = \{p, H_{\text{primary}}\}, \\
&\dot{z}_a = \{z_a, H_{\text{primary}}\} = \{p_a, H_{\text{primary}}\}, \\
&\dot{\Lambda}^{jj} = \{\Lambda^{jj}, H_{\text{primary}}\} = \{\Pi^{jj}, H_{\text{primary}}\}.
\end{aligned} \tag{855}$$

E.1.1 Secondary Constraint $\dot{z}$

I. Calculate

$$\begin{aligned}
\dot{z} &= \{z, H_{\text{primary}}\} = \{p, H_{\text{primary}}\} \\
&= \int_\chi \mathrm{d}^3x\,\{p, h_{\text{primary}}\} = \int_\chi \mathrm{d}^3x\,\{p, \nu z + \nu^b z_b + \sum_{j=1}^{3}\mu_{jj}\Lambda^{jj} + nc^{\text{tot}} + n^b c^{\text{tot}}_b\}
\end{aligned} \tag{856}$$

1. $\int_\chi \mathrm{d}^3x\,\{p, \nu z\} = \int_\chi \mathrm{d}^3x\,\nu\{p,p\} = 0$

2. $\int_\chi \mathrm{d}^3x\,\{p, \nu^b z_b\} = \int_\chi \mathrm{d}^3x\,\nu^b\{p,p_b\} = 0$

3. $\int_\chi \mathrm{d}^3x\,\{p, \sum_{j=1}^{3}\mu_{jj}\Lambda^{jj}\} = \int_\chi \mathrm{d}^3x\,\sum_{j=1}^{3}\mu_{jj}\{p,\Pi^{jj}\} = 0$

4. $\int_\chi \mathrm{d}^3x\,\{p, nc^{\text{tot}}\} = \int_\chi \mathrm{d}^3x\,\{p, n\,(c^{\text{geo}} + c^\varphi)\}$
   $= \int_\chi \mathrm{d}^3x \left(c^{\text{geo}} \underbrace{\{p,n\}}_{-\delta^{(3)}(x,y)} + c^\varphi \underbrace{\{p,n\}}_{-\delta^{(3)}(x,y)} \right) = -\int_\chi \mathrm{d}^3x\, c^{\text{tot}}\delta^{(3)}(x,y) = -c^{\text{tot}}$

5. $\int_\chi \mathrm{d}^3x\,\{p, n^b c^{\text{tot}}_b\} = \int_\chi \mathrm{d}^3x\,\{p, n^b\,(c^{\text{geo}}_b + c^\varphi_b)\} = \int_\chi \mathrm{d}^3x\, n^b\{p, \pi_I\varphi^I_{,b}\} = 0$

   In summary we obtain

$$\dot{z} = \{p, H_{\text{primary}}\} = -c^{\text{tot}}. \tag{857}$$

E.1.2 Secondary Constraint $\dot{z}_a$

II. Calculate

$$\begin{aligned}\dot{z}_a &= \{z_a, H_{\text{primary}}\} = \{p_a, H_{\text{primary}}\} \\ &= \int\limits_\chi \mathrm{d}^3x\, \{p_a, h_{\text{primary}}\} = \int\limits_\chi \mathrm{d}^3x\, \{p_a, \nu z + \nu^b z_b + \sum_{j=1}^{3} \mu_{jj}\Lambda^{jj} + nc^{\text{tot}} + n^b c_b^{\text{tot}}\}\end{aligned} \tag{858}$$

1. $\int\limits_\chi \mathrm{d}^3x\, \{p_a, \nu z\} = \int\limits_\chi \mathrm{d}^3x\, \nu\{p_a, p\} = 0$

2. $\int\limits_\chi \mathrm{d}^3x\, \{p_a, \nu^b z_b\} = \int\limits_\chi \mathrm{d}^3x\, \nu^b\{p_a, p_b\} = 0$

3. $\int\limits_\chi \mathrm{d}^3x\, \{p_a, \sum\limits_{j=1}^{3} \mu_{jj}\Lambda^{jj}\} = \int\limits_\chi \mathrm{d}^3x\, \sum\limits_{j=1}^{3} \mu_{jj}\{p_a, \Pi^{jj}\} = 0$

4. $\int\limits_\chi \mathrm{d}^3x\, \{p_a, nc^{\text{tot}}\} = \int\limits_\chi \mathrm{d}^3x\, \{p_a, n\,(c^{\text{geo}} + c^{\varphi})\} = 0$

5. $\int\limits_\chi \mathrm{d}^3x\, \{p_a, nc^{\text{tot}}\} = \int\limits_\chi \mathrm{d}^3x\, \{p_a, n^b\,(c_b^{\text{geo}} + c_b^{\varphi})\}$
$= \int\limits_\chi \mathrm{d}^3x \left(c_b^{\text{geo}} \underbrace{\{p_a, n^b\}}_{-\delta_a^b\delta^{(3)}(x,y)} + c_b^{\varphi} \underbrace{\{p_a, n^b\}}_{-\delta_a^b\delta^{(3)}(x,y)} \right) = -\int\limits_\chi \mathrm{d}^3x\, c_a^{\text{tot}}\delta^{(3)}(x,y) = -c_a^{\text{tot}}$

In summary we obtain

$$\dot{z}_a = \{p_a, H_{\text{primary}}\} = -c_a^{\text{tot}}. \tag{859}$$

E.1.3 Secondary Constraint $\dot{\Lambda}^{jj}$

III. Calculate

$$\begin{aligned}\dot{\Lambda}^{jj} &= \{\Lambda^{jj}, H_{\text{primary}}\} = \{\Pi^{jj}, H_{\text{primary}}\} \\ &= \int\limits_\chi \mathrm{d}^3x\, \{\Pi^{jj}, h_{\text{primary}}\} = \int\limits_\chi \mathrm{d}^3x\, \{\Pi^{jj}, \nu z + \nu^b z_b + \rho^k\Phi_k + \sum_{k=1}^{3} \mu_{kk}\Lambda^{kk} + nc^{tot} + n^b c_b^{tot}\}\end{aligned} \tag{860}$$

1. $\int\limits_\chi \mathrm{d}^3x\, \{\Pi^{jj}, \nu z\} = \int\limits_\chi \mathrm{d}^3x\, \nu\{\Pi^{jj}, p\} = 0$

2. $\int\limits_\chi \mathrm{d}^3x\, \{\Pi^{jj}, \nu^b z_b\} = \int\limits_\chi \mathrm{d}^3x\, \nu^b\{\Pi^{jj}, p_b\} = 0$

3. $\int\limits_\chi \mathrm{d}^3x\, \{\Pi^{jj}, \sum\limits_{k=1}^{3} \mu_{kk}\Lambda^{kk}\} = \int\limits_\chi \mathrm{d}^3x\, \sum\limits_{k=1}^{3} \mu_{kk}\{\Pi^{jj}, \Pi^{kk}\} = 0$

4. $\int\limits_\chi \mathrm{d}^3x\, \{\Pi^{jj}, nc^{\text{tot}}\} = \int\limits_\chi \mathrm{d}^3x\, \{\Pi^{jj}, n\,(c^{\text{geo}} + c^{\varphi})\} = \int\limits_\chi \mathrm{d}^3x \left(n \underbrace{\{\Pi^{jj}, c^{\text{geo}}\}}_{=0} + n\{\Pi^{jj}, c^{\varphi}\} \right)$
$= \int\limits_\chi \mathrm{d}^3x\, n\{\Pi^{jj}, \frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} + \sum\limits_{k=1}^{3} \left(\frac{(M^{-1})^{kk}\pi_k\pi_k}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}M_{kk}\varphi^k_{,a}\varphi^k_{,b} \right)\}$
$= \int\limits_\chi \mathrm{d}^3x \left(n \sum\limits_{k=1}^{3} \frac{\pi_k\pi_k}{2\sqrt{q}}\{\Pi^{jj}, (M^{-1})^{kk}\} + n \sum\limits_{k=1}^{3} \frac{1}{2}\sqrt{q}q^{ab}\varphi^k_{,a}\varphi^k_{,b} \underbrace{\{\Pi^{jj}, M_{kk}\}}_{-\delta_k^j\delta^{(3)}(x,y)} \right)$

$$
\begin{aligned}
&= \int_\chi \mathrm{d}^3x \left(-n \sum_{k=1}^{3} \tfrac{\pi_k \pi_k}{2\sqrt{q}} (M^{-1})^{k\ell}(M^{-1})^{k\ell} \underbrace{\{\Pi^{jj}, M_{\ell\ell}\}}_{-\delta^j_\ell \delta^{(3)}(x,y)} - n\tfrac{1}{2}\sqrt{q} q^{ab}\varphi^j_{,a}\varphi^j_{,b}\delta^{(3)}(x,y) \right) \\
&= \int_\chi \mathrm{d}^3x \left(n \sum_{k=1}^{3} \tfrac{(M^{-1})^{kj}(M^{-1})^{kj}\pi_k\pi_k}{2\sqrt{q}} \delta^{(3)}(x,y) - n\tfrac{1}{2}\sqrt{q} q^{ab}\varphi^j_{,a}\varphi^j_{,b}\delta^{(3)}(x,y) \right) \\
&= \int_\chi \mathrm{d}^3x \, n \left[\tfrac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j}{2\sqrt{q}} - \tfrac{1}{2}\sqrt{q} q^{ab}\varphi^j_{,a}\varphi^j_{,b} \right] \delta^{(3)}(x,y) \\
&= n \left[\tfrac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j}{2\sqrt{q}} - \tfrac{1}{2}\sqrt{q} q^{ab}\varphi^j_{,a}\varphi^j_{,b} \right]
\end{aligned}
$$

5. $\int_\chi \mathrm{d}^3x \, \{\Pi^{jj}, n^b c^{\mathrm{tot}}_b\} = \int_\chi \mathrm{d}^3x \, n^b \{\Pi^{jj}, c^{\mathrm{geo}}_b + \pi_0\varphi^0_{,b} + \sum_{j=1}^{3} \pi_j \varphi^j_{,b}\} = 0$

In the calculation above we used that

$$
\begin{aligned}
0 = \delta\delta^i_j &= \delta\left((M^{-1})^{ik} M_{kj}\right) = \delta(M^{-1})^{ik} M_{kj} + (M^{-1})^{ik}\delta M_{kj} \\
&\Leftrightarrow \delta(M^{-1})^{ik} M_{kj} = -(M^{-1})^{ik}\delta M_{kj},
\end{aligned}
$$

multiplication with $(M^{-1})^{j\ell}$ from the right side gives

$$
\begin{aligned}
&\delta(M^{-1})^{ik}\delta^\ell_k = -(M^{-1})^{ik}\delta M_{kj}(M^{-1})^{j\ell} \\
&\Rightarrow M^{i\ell} = -(M^{-1})^{ik}(M^{-1})^{j\ell}\delta M_{kj}
\end{aligned}
$$

In summary we obtain

$$
\dot{\Lambda}^{jj} = \{\Pi^{jj}, H_{\mathrm{primary}}\} = \frac{n}{2}\left[\frac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j}{\sqrt{q}} - \sqrt{q} q^{ab}\varphi^j_{,a}\varphi^j_{,b} \right] =: c^{jj}. \tag{861}
$$

E.2 Summary Secondary Constraints

The constraint stability analysis of the primary constraints z, z_a and Λ^{jj} leads to

$$
\begin{aligned}
\dot{z} &= \{p, H_{\mathrm{primary}}\} = -c^{\mathrm{tot}}, \qquad (862)\\
\dot{z}_a &= \{p_a, H_{\mathrm{primary}}\} = -c^{\mathrm{tot}}_a, \\
\dot{\Lambda}^{jj} &= \{\Pi^{jj}, H_{\mathrm{primary}}\} = \frac{n}{2}\left[\frac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j}{2\sqrt{q}} - \sqrt{q} q^{ab}\varphi^j_{,a}\varphi^j_{,b} \right].
\end{aligned}
$$

We realize that we obtain three more secondary constraints that we denote by c^{jj} which are given by

$$
c^{jj} := \frac{n}{2}\left[\frac{(M^{-1})^{jk}(M^{-1})^{j\ell}\pi_k\pi_\ell}{\sqrt{q}} - \sqrt{q} q^{ab}\varphi^j_{,a}\varphi^j_{,b} \right]. \tag{863}
$$

In order to ensure that the primary constraints z, z_a and Λ^{jj} are stable we require c^{tot}, c^{tot}_a and c^{jj} to be secondary constraints.

E.3 Constraint Stability Analysis - Tertiary Constraints

Now given the set of secondary constraints $\{c^{\mathrm{tot}}, c^{\mathrm{tot}}_a, c^{jj}\}$ we need to compute whether these constraints are stable with respect to H_{primary} or whether tertiary constraints occur. For writing comfort we define $M^{00} := (M^{-1})^{00} := \mathbb{1}_3$ and $I, J = 0, 1, 2, 3$.

E.3.1 Tertiary Constraint $\dot{c}^{tot}(n)$

I. Calculate

We define the smeared constraint $c^{\text{tot}}(n) := \int\limits_{\chi} \mathrm{d}^3x\, n(x) c^{\text{tot}}(x)$ and calculate

$$
\begin{aligned}
&\{c^{tot}(n), H_{\text{primary}}\} \qquad (864)\\
&= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\{n(x)c^{\text{tot}}(x), \nu(y)z(y)\} + \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\{n(x)c^{\text{tot}}(x), \nu^b(y)z_b(y)\}\\
&+ \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\{n(x)c^{\text{tot}}(x), \sum_{k=1}^{3}\mu_{kk}(y)\Lambda^{kk}(y)\}\\
&+ \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\{n(x)c^{\text{tot}}(x), n'(y)c^{\text{tot}}(y)\} + \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\{n(x)c^{\text{tot}}(x), n'^b(y)c^{\text{tot}}_b(y)\}.
\end{aligned}
$$

For the single terms we get the expressions:

1. $\int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\{n(x)c^{\text{tot}}(x), \nu(y)z(y)\}$
$= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\left(\{n(x)c^{\text{geo}}(x), \nu(y)p(y)\} + \{n(x)c^{\varphi}(x), \nu(y)p(y)\}\right)$
$= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\left(\nu(y)c^{\text{geo}}(x)\underbrace{\{n(x), p(y)\}}_{\delta^{(3)}(x,y)} + \nu(y)c^{\varphi}(x)\underbrace{\{n(x), p(y)\}}_{\delta^{(3)}(x,y)}\right)$
$= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\nu(y)c^{\text{tot}}(x)\delta^{(3)}(x,y) = \int\limits_{\chi}\mathrm{d}^3x\,\nu(x)c^{\text{tot}}(x) = c^{\text{tot}}(\nu)$

2. $\int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\{n(x)c^{\text{tot}}(x), \nu^b(y)z_b(y)\}$
$= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\left(\{n(x)c^{\text{geo}}(x), \nu^b(y)p_b(y)\} + \{n(x)c^{\varphi}(x), \nu^b(y)p_b(y)\}\right)$
$= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\left(\nu(y)c^{\text{geo}}(x)\underbrace{\{n(x), p_b(y)\}}_{=0} + \nu(y)c^{\varphi}(x)\underbrace{\{n(x), p_b(y)\}}_{=0}\right) = 0$

3. $\int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\{n(x)c^{tot}(x), \mu_{kk}(y)\Pi^{kk}(y)\}$
$= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\left(\underbrace{\{n(x)c^{\text{geo}}(x), \sum_{k=1}^{3}\mu_{kk}(y)\Pi^{kk}(y)\}}_{=0} + \{n(x)c^{\varphi}(x), \sum\limits_{k=1}^{3}\mu_{kk}(y)\Pi^{kk}(y)\}\right)$
$= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\sum\limits_{k=1}^{3}\mu_{kk}(y)n(x)\{\left[\frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} + \sum\limits_{j=1}^{3}\left(\frac{(M^{-1})^{jj}\pi_j\pi_j}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}M_{jj}\varphi^j_{,a}\varphi^j_{,b}\right)\right](x), \Pi^{kk}(y)\}$
$= \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\sum\limits_{k=1}^{3}\sum\limits_{j=1}^{3}\mu_{kk}(y)n(x)\left(\left[\frac{\pi_j\pi_j}{2\sqrt{q}}\right](x)\{(M^{-1})^{jj}(x), \Pi^{kk}(y),\} + \left[\frac{1}{2}\sqrt{q}q^{ab}\varphi^j_{,a}\varphi^j_{,b}\right](x)\underbrace{\{M_{jj}(x), \Pi^{kk}(y)\}}_{\delta^k_j\delta^{(3)}(x,y)}\right)$
$= -\int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\sum\limits_{k=1}^{3}\sum\limits_{j=1}^{3}\mu_{kk}(y)n(x)\left[\frac{\pi_j\pi_j}{2\sqrt{2}}(M^{-1})^{j\ell}(M^{-1})^{j\ell}\right](x)\underbrace{\{M_{\ell\ell}(x), \Pi^{kk}(y)\}}_{\delta^k_\ell\delta^{(3)}(x,y)}$
$+ \int\limits_{\chi}\mathrm{d}^3x \int\limits_{\chi}\mathrm{d}^3y\,\sum\limits_{j=1}^{3}\mu_{jj}(y)n(x)\left[\frac{1}{2}\sqrt{q}q^{ab}\varphi^j_{,a}\varphi^j_{,b}\right](x)\delta^{(3)}(x,y)$

$$= -\int_\chi \mathrm{d}^3x \sum_{k=1}^{3}\sum_{j=1}^{3} \mu_{kk}(x)n(x)\left[\frac{\pi_j\pi_j}{2\sqrt{q}}(M^{-1})^{jk}(M^{-1})^{jk}\right](x) + \int_\chi \mathrm{d}^3x \sum_{j=1}^{3}\mu_{jj}(x)n(x)\left[\frac{1}{2}\sqrt{q}q^{ab}\varphi^j_{,a}\varphi^j_{,b}\right](x)$$
$$= \int_\chi \mathrm{d}^3x \sum_{j=1}^{3}\mu_{jj}(x)\left[-\frac{n}{2}\left[\frac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j}{\sqrt{q}} - \sqrt{q}q^{ab}\varphi^j_{,a}\varphi^j_{,b}\right]\right](x)$$
$$= -\int_\chi \mathrm{d}^3x \sum_{j=1}^{3}\mu_{jj}(x)c^{jj}(x) := -c(\mu)$$

Since the fourth and the fifth term are rather lenghty, we display them here separately divided again into subterms.

4. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\mathrm{tot}}(x), n'(y)c^{\mathrm{tot}}(y)\}$
$$= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\mathrm{geo}}(x), n'(y)c^{\mathrm{tot}}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\varphi}(x), n'(y)c^{\mathrm{tot}}(y)\}$$
$$= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\mathrm{geo}}(x), n'(y)c^{\mathrm{geo}}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\mathrm{geo}}(x), n'(y)c^{\varphi}(y)\}$$
$$+ \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\varphi}(x), n'(y)c^{\mathrm{geo}}(y)\} + \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\varphi}(x), n'(y)c^{\varphi}(y)\}$$

4.1. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\mathrm{geo}}(x), n'(y)c^{\mathrm{geo}}(y)\} = \{c^{\mathrm{geo}}(n), c^{\mathrm{geo}}(n')\} = \vec{c}^{\mathrm{geo}}\left(q^{-1}\left[n\mathrm{d}n' - n'\mathrm{d}n\right]\right)$

4.2. $\int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \,\{n(x)c^{\mathrm{geo}}(x), n'(y)c^{\varphi}(y)\}$
$$= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \, n(x)n'(y)\{\left[\frac{2}{\kappa\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right)p^{ab}p^{cd} - \sqrt{q}R^{(3)}\right](x),$$
$$\left[\sum_{J=0}^{3}\left(\frac{(M^{-1})^{JJ}\pi_J\pi_J}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ef}M_{JJ}\varphi^J_{,e}\varphi^J_{,f}\right)\right](y)\}$$
$$= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \, n(x)n'(y)\left[\frac{2}{\kappa\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right)\right](x)$$
$$\left(\left[\sum_{J=0}^{3}\frac{(M^{-1})^{JJ}\pi_J\pi_J}{2}\right](y)\{p^{ab}(x)p^{cd}(x), \frac{1}{\sqrt{q}}(y)\} + \left[\sum_{J=0}^{3}\frac{1}{2}M_{JJ}\varphi^J_{,e}\varphi^J_{f}\right](y)\{p^{ab}(x)p^{cd}(x), \sqrt{q}(y)q^{ef}(y)\}\right)$$
$$= \int_\chi \mathrm{d}^3x \int_\chi \mathrm{d}^3y \, n(x)n'(y)\left[\frac{2}{\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right)\right](x)$$
$$\left(\left[\sum_{J=0}^{3}\frac{(M^{-1})^{JJ}\pi_J\pi_J}{2}\right](y)\left(p^{ab}(x)\left[\frac{1}{2}\frac{1}{\sqrt{q}}q^{cd}\right](y) + p^{cd}(x)\left[\frac{1}{2}\frac{1}{\sqrt{q}}q^{ab}\right](y)\right)\right.$$
$$- \left[\sum_{J=0}^{3}\frac{1}{2}M_{JJ}\varphi^J_{,e}\varphi^J_{f}\right](y)\left(p^{ab}(x)\left[\frac{1}{2}\sqrt{q}q^{cd}q^{ef}\right](y) + p^{cd}(x)\left[\frac{1}{2}\sqrt{q}q^{ab}q^{ef}\right](y)\right)$$
$$\left. + \left[\sum_{J=0}^{3}\frac{1}{2}M_{JJ}\varphi^J_{,e}\varphi^J_{f}\right](y)\left(p^{ab}(x)\left[\sqrt{q}q^{ec}q^{fd}\right](y) + p^{cd}(x)\left[\sqrt{q}q^{ea}q^{fb}\right](y)\right)\right)\delta^{(3)}(x,y)$$
$$= \int_\chi \mathrm{d}^3x \, nn'\left[\frac{1}{\sqrt{q}}\left(q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right)\right]$$
$$\left(\left[\sum_{J=0}^{3}\frac{(M^{-1})^{JJ}\pi_J\pi_J}{2\sqrt{q}}\right]\left(p^{ab}q^{cd} + p^{cd}q^{ab}\right) - \left[\sum_{J=0}^{3}\frac{1}{2}M_{JJ}\sqrt{q}q^{ef}\varphi^J_{,e}\varphi^J_{,f}\right]\left(p^{ab}q^{cd} + p^{cd}q^{ab}\right)\right.$$
$$\left. + 2\left[\sum_{J=0}^{3}\frac{1}{2}M_{JJ}\sqrt{q}\varphi^J_{,e}\varphi^J_{,f}\right]\left(p^{ab}q^{ec}q^{fd} + p^{cd}q^{ea}q^{fb}\right)\right)$$
$$= \int_\chi \mathrm{d}^3x \, nn'\frac{1}{\sqrt{q}}\left(\left[\sum_{J=0}^{3}\frac{(M^{-1})^{JJ}\pi_J\pi_J}{2\sqrt{q}}\right]\left(-q_{ab}p^{ab}\right) - \left[\sum_{J=0}^{3}\frac{1}{2}M_{JJ}\sqrt{q}q^{ef}\varphi^J_{,e}\varphi^J_{,f}\right]\left(-q_{ab}p^{ab}\right)\right.$$
$$\left. + 2\left[\sum_{J=0}^{3}\frac{1}{2}M_{JJ}\sqrt{q}\varphi^J_{,e}\varphi^J_{,f}\right]\left(2p^{ef} - q_{ab}p^{ab}q^{ef}\right)\right)$$

$$= -nn'\tfrac{1}{\sqrt{q}}\Bigg(\left[\sum_{J=0}^{3}\tfrac{(M^{-1})^{JJ}\pi_J\pi_J}{2\sqrt{q}}\right]q_{ab}p^{ab} - \left[\sum_{J=0}^{3}\tfrac{1}{2}M_{JJ}\sqrt{q}q^{ef}\varphi^J_{,e}\varphi^J_{,f}\right]q_{ab}p^{ab}$$
$$+ 4\left[\sum_{J=0}^{3}\tfrac{1}{2}M_{JJ}\sqrt{q}\varphi^J_{,e}\varphi^J_{,f}\right]p^{ef}\Bigg)$$
$$= -\int_\chi \mathrm{d}^3x\, nn'\tfrac{1}{\sqrt{q}}c^\varphi q_{ab}p^{ab} + \int_\chi \mathrm{d}^3x\, nn'\tfrac{4}{\sqrt{q}}\left[\sum_{J=0}^{3}\tfrac{1}{2}M_{JJ}\sqrt{q}\varphi^J_{,e}\varphi^J_{,f}\right]p^{ef}$$

4.3. $\int_\chi \mathrm{d}^3x\int_\chi \mathrm{d}^3y\,\{n(x)c^\varphi(x), n'(y)c^{\mathrm{geo}}(y)\}$
$$= \int_\chi \mathrm{d}^3x\, nn'\tfrac{1}{\sqrt{q}}c^\varphi q_{ab}p^{ab} - \int_\chi \mathrm{d}^3x\, nn'\tfrac{4}{\sqrt{q}}\left[\sum_{J=0}^{3}\tfrac{1}{2}M_{JJ}\sqrt{q}\varphi^J_{,e}\varphi^J_{f}\right]p^{ef}$$

We used that:

$$\{p^{ab}(x)p^{cd}(x), \frac{1}{\sqrt{q}}(y)\}$$
$$= p^{ab}(x)\{p^{cd}(x), \frac{1}{\sqrt{q}}(y)\} + \{p^{ab}(x), \frac{1}{\sqrt{q}}(y)\}p^{cd}(x)$$
$$= p^{ab}(x)\left[-\frac{1}{2}\frac{1}{\sqrt{q}}q^{gh}\right](y)\{p^{cd}(x), q_{gh}(y)\} + p^{cd}(x)\left[-\frac{1}{2}\frac{1}{\sqrt{q}}q^{gh}\right](y)\{p^{ab}(x), q_{gh}(y)\}$$
$$= -\kappa\delta^c_{(g}\delta^d_{h)}\, p^{ab}(x)\left[-\frac{1}{2}\frac{1}{\sqrt{q}}q^{gh}\right](y)\delta^{(3)}(x,y) - \kappa\delta^a_{(g}\delta^b_{h)}\, p^{cd}(x)\left[-\frac{1}{2}\frac{1}{\sqrt{q}}q^{gh}\right](y)\delta^{(3)}(x,y)$$
$$= \kappa\left(p^{ab}(x)\left[\frac{1}{2}\frac{1}{\sqrt{q}}q^{cd}\right](y) + p^{cd}(x)\left[\frac{1}{2}\frac{1}{\sqrt{q}}q^{ab}\right](y)\right)\delta^{(3)}(x,y)$$

$$\{p^{ab}(x)p^{cd}(x), \sqrt{q}(y)q^{ef}(y)\}$$
$$= p^{ab}(x)\{p^{cd}(x), \sqrt{q}(y)q^{ef}(y)\} + p^{cd}(x)\{p^{ab}(x), \sqrt{q}(y)q^{ef}(y)\}$$
$$= p^{ab}(x)q^{ef}(y)\{p^{cd}(x), \sqrt{q}(y)\} + p^{cd}(x)q^{ef}(y)\{p^{ab}(x), \sqrt{q}(y)\}$$
$$+ p^{ab}(x)\sqrt{q}(y)\{p^{cd}(x), q^{ef}(y)\} + p^{cd}(x)\sqrt{q}(y)\{p^{ab}(x), q^{ef}(y)\}$$
$$= p^{ab}(x)\left[\frac{1}{2}\sqrt{q}q^{gh}q^{ef}\right](y)\{p^{cd}(x), q_{gh}(y)\} + p^{cd}(x)\left[\frac{1}{2}\sqrt{q}q^{gh}q^{ef}\right](y)\{p^{ab}(x), q_{gh}(y)\}$$
$$- p^{ab}(x)\left[\sqrt{q}q^{eg}q^{fh}\right](y)\{p^{cd}(x), q_{gh}(y)\} - p^{cd}(x)\left[\sqrt{q}q^{eg}q^{fh}\right](y)\{p^{ab}(x), q_{gh}(y)\}$$
$$= -\kappa\delta^c_{(g}\delta^d_{h)}p^{ab}(x)\left[\frac{1}{2}\sqrt{q}q^{gh}q^{ef}\right](y)\delta^{(3)}(x,y) - \kappa\delta^a_{(g}\delta^b_{h)}p^{cd}(x)\left[\frac{1}{2}\sqrt{q}q^{gh}q^{ef}\right](y)\delta^{(3)}(x,y)$$
$$+ \kappa\delta^c_{(g}\delta^d_{h)}p^{ab}(x)\left[\sqrt{q}q^{eg}q^{fh}\right](y)\delta^{(3)}(x,y) + \kappa\delta^a_{(g}\delta^b_{h)}p^{cd}(x)\left[\sqrt{q}q^{eg}q^{fh}\right](y)\delta^{(3)}(x,y)$$
$$= -\kappa\left(p^{ab}(x)\left[\frac{1}{2}\sqrt{q}q^{cd}q^{ef}\right](y) + p^{cd}(x)\left[\frac{1}{2}\sqrt{q}q^{ab}q^{ef}\right](y)\right)\delta^{(3)}(x,y)$$
$$+ \kappa\left(p^{ab}(x)\left[\sqrt{q}q^{ec}q^{fd}\right](y) + p^{cd}(x)\left[\sqrt{q}q^{ea}q^{fb}\right](y)\right)\delta^{(3)}(x,y)$$

4.4. $\int_\chi \mathrm{d}^3x\int_\chi \mathrm{d}^3y\,\{n(x)c^\varphi(x), n'(y)c^\varphi(y)\}$
$$= \int_\chi \mathrm{d}^3x\int_\chi \mathrm{d}^3y\,\{n(x)\left[\sum_{J=0}^{3}\left(\tfrac{(M^{-1})^{JJ}\pi_J\pi_J}{2\sqrt{q}} + \tfrac{1}{2}\sqrt{q}q^{ab}M_{JJ}\varphi^J_{,a}\varphi^J_{b}\right)\right](x),$$

$$\begin{aligned}
&n'(y)\left[\sum_{I=0}^{3}\left(\tfrac{(M^{-1})^{II}\pi_I\pi_I}{2\sqrt{q}}+\tfrac{1}{2}\sqrt{q}q^{cd}M_{II}\varphi^I_{,c}\varphi^I_{,d}\right)\right](y)\}\\
&=\int_\chi d^3x\int_\chi d^3y\, n(x)n'(y)\left[\sum_{J=0}^{3}\tfrac{(M^{-1})^{JJ}}{2\sqrt{q}}\right](x)\left[\sum_{I=0}^{3}\tfrac{1}{2}\sqrt{q}q^{cd}M_{II}\right](y)\{\pi_J(x)\pi_J(x),\varphi^I_{,c}(y)\varphi^I_{,d}(y)\}\\
&-\int_\chi d^3x\int_\chi d^3y\, n(x)n'(y)\left[\sum_{I=0}^{3}\tfrac{(M^{-1})^{II}}{2\sqrt{q}}\right](y)\left[\sum_{J=0}^{3}\tfrac{1}{2}\sqrt{q}q^{ab}M_{JJ}\right](x)\{\pi_I(y)\pi_I(y),\varphi^J_{,a}(x)\varphi^J_{,b}(x)\}\\
&=-4\int_\chi d^3x\int_\chi d^3y\left[n\sum_{J=0}^{3}\tfrac{(M^{-1})^{JJ}}{2\sqrt{q}}\right](x)\left[n'\sum_{I=0}^{3}\tfrac{1}{2}\sqrt{q}q^{cd}M_{II}\right](y)\pi_J(x)\varphi^I_{,c}(y)\delta^I_J\tfrac{\partial}{\partial y^d}\delta^{(3)}(x,y)\\
&+4\int_\chi d^3x\int_\chi d^3y\left[n'\sum_{I=0}^{3}\tfrac{(M^{-1})^{II}}{2\sqrt{q}}\right](y)\left[n\sum_{J=0}^{3}\tfrac{1}{2}\sqrt{q}q^{ab}M_{JJ}\right](x)\pi_I(y)\varphi^J_{,a}(x)\delta^J_I\tfrac{\partial}{\partial x^b}\delta^{(3)}(x,y)\\
&=\int_\chi d^3x\sum_{J=0}^{3}\left[n\tfrac{(M^{-1})^{JJ}\pi_J}{\sqrt{q}}\right]\left[n'\sqrt{q}q^{ab}M_{JJ}\varphi^J_{,a}\right]_{,b}-\int_\chi d^3x\sum_{J=0}^{3}\left[n'\tfrac{(M^{-1})^{JJ}\pi_J}{\sqrt{q}}\right]\left[n\sqrt{q}q^{ab}M_{JJ}\varphi^J_{,a}\right]_{,b}\\
&=\int_\chi d^3x\left(n\,n'_{,b}-n'\,n_{,b}\right)\sum_{J=0}^{3}\tfrac{(M^{-1})^{JJ}\pi_J}{\sqrt{q}}\sqrt{q}q^{ab}M_{JJ}\varphi^J_{,a}\\
&=\int_\chi d^3x\left(n\,n'_{,b}-n'\,n_{,b}\right)q^{ab}\sum_{J=0}^{3}\pi_J\varphi^J_{,a}=\int_\chi d^3x\left(n\,n'_{,b}-n'\,n_{,b}\right)q^{ab}c^\varphi_a\\
&=\vec{c}^\varphi\left(q^{-1}\left[n\,dn'-n'\,dn\right]\right)
\end{aligned}$$

We used that:

$$\begin{aligned}
&\{\pi_I(y)\pi_I(y),\varphi^J_{,a}(x)\varphi^J_{,b}(x)\}=2\pi_I(y)\{\pi_I(y),\varphi^J_{,a}(x)\varphi^J_{,b}(x)\}\\
&\overset{q^{ab}\equiv q^{ba}}{=}4\pi_I(y)\varphi^J_{,a}(x)\{\pi_I(y),\varphi^J_{,b}(x)\}=-4\pi_I(y)\varphi^J_{,a}(x)\delta^J_I\frac{\partial}{\partial x^b}\delta^{(3)}(x,y)
\end{aligned}$$

We see that the terms 4.2. and 4.3. cancel each other so that in the end we are left with

4. $\int_\chi d^3x\int_\chi d^3y\,\{n(x)c^{\text{tot}}(x),n'(y)c^{\text{tot}}(y)\}$
$=\vec{c}^{\text{geo}}\left(q^{-1}\left[n\,d\,n'-n'dn\right]\right)+\vec{c}^\varphi\left(q^{-1}\left[n\,dn'-n'\,dn\right]\right)=\vec{c}^{\text{tot}}\left(q^{-1}\left[n\,d\,n'-n'dn\right]\right)$

5. $\int_\chi d^3x\int_\chi d^3y\,\{n(x)c^{\text{tot}}(x),n'^b(y)c^{\text{tot}}_b(y)\}$
$=\int_\chi d^3x\int_\chi d^3y\,\{n(x)c^{\text{geo}}(x),n'^b(y)c^{\text{geo}}_b(y)\}+\int_\chi d^3x\int_\chi d^3y\,\{n(x)c^{\text{geo}}(x),n'^b(y)c^\varphi_b(y)\}$
$+\int_\chi d^3x\int_\chi d^3y\,\{n(x)c^\varphi(x),n'^b(y)c^{\text{geo}}_b(y)\}+\int_\chi d^3x\int_\chi d^3y\,\{n(x)c^\varphi(x),n'^b(y)c^\varphi_b(y)\}$

5.1. $\int_\chi d^3x\int_\chi d^3y\,\{n(x)c^{\text{geo}}(x),n'^b(y)c^{\text{geo}}_b(y)\}=\{c^{\text{geo}}(n),\vec{c}^{\text{geo}}(\vec{n}')\}=-c^{\text{geo}}(\pounds_{\vec{n}'}n)$

5.2. $\int_\chi d^3x\int_\chi d^3y\,\{n(x)c^{\text{geo}}(x),n'^b(y)c^\varphi_b(y)\}=0$

In the following calculation we are going to define

$$f[\pi,M](x):=\frac{1}{2}\sum_{J=0}^{3}(M^{-1})^{JJ}\pi_J\pi_J,\quad k_{ab}[\varphi,M](x):=\frac{1}{2}\sum_{J=0}^{3}M_{JJ}\varphi^J_{,a}\varphi^J_b.\tag{865}$$

Notice that $c^\varphi=\sum_{J=0}^{3}\left(\frac{(M^{-1})^{JJ}\pi_J\pi_J}{2\sqrt{q}}+\frac{1}{2}\sqrt{q}q^{ab}M_{JJ}\varphi^J_{,a}\varphi^J_b\right)=\frac{f}{\sqrt{q}}+\sqrt{q}q^{ab}k_{ab}$.

5.3. $\int\limits_\chi d^3x \int\limits_\chi d^3y\, \{n(x)c^\varphi(x), n'^b(y)c_b^{\text{geo}}(y)\}$

$$= \int\limits_\chi d^3x \int\limits_\chi d^3y\, \{n(x)\left[\sum_{J=0}^{3}\left(\frac{(M^{-1})^{JJ}\pi_J\pi_J}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}M_{JJ}\varphi^J_{,a}\varphi^J_{b}\right)\right](x), \frac{1}{\kappa}\left[p^{cd}\left(\pounds_{\vec{n}'}q\right)_{cd}\right]\}$$
$$=: \int\limits_\chi d^3x \int\limits_\chi d^3y\, \{\left[nf\frac{1}{\sqrt{q}} + \sqrt{q}q^{ab}k_{ab}\right](x), \frac{1}{\kappa}\left[p^{cd}\left(\pounds_{\vec{n}'}q\right)_{cd}\right]\}$$
$$= \frac{1}{\kappa}\int\limits_\chi d^3x \int\limits_\chi d^3y\, [nf](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\{\tfrac{1}{\sqrt{q}}(x), p^{cd}(y)\}$$
$$+ \frac{1}{\kappa}\int\limits_\chi d^3x \int\limits_\chi d^3y\, [nk_{ab}](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\{\sqrt{q}(x)q^{ab}(x), p^{cd}(y)\}$$
$$= \frac{1}{\kappa}\int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[-\tfrac{1}{2}\tfrac{1}{\sqrt{q}}q^{gh}nf\right](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\{q_{gh}(x), p^{cd}(y)\}$$
$$+ \frac{1}{\kappa}\int\limits_\chi d^3x \int\limits_\chi d^3y\, [nk_{ab}](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\{\sqrt{q}(x)q^{ab}(x), p^{cd}(y)\}$$
$$= \int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[-\tfrac{1}{2}\tfrac{1}{\sqrt{q}}q^{gh}nf\right](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\delta^c_{(g}\delta^d_{h)}\delta^{(3)}(x,y)$$
$$+\frac{1}{\kappa}\int\limits_\chi d^3x \int\limits_\chi d^3y\, [nk_{ab}](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\left(\sqrt{q}(x)\{q^{ab}(x), p^{cd}(y)\} + q^{ab}(x)\{\sqrt{q}(x), p^{cd}(y)\}\right)$$
$$= \int\limits_\chi d^3x\, \left[nf\left(\pounds_{\vec{n}'}\tfrac{1}{\sqrt{q}}\right)_{cd}\right](x)$$
$$- \frac{1}{\kappa}\int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[\sqrt{q}q^{ag}q^{bh}nk_{ab}\right](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\{q_{gh}(x), p^{cd}(y)\}$$
$$+ \frac{1}{\kappa}\int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[\tfrac{1}{2}\sqrt{q}q^{gh}q^{ab}nk_{ab}\right](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\{q_{gh}(x), p^{cd}(y)\}$$
$$= \int\limits_\chi d^3x\, \left[nf\left(\pounds_{\vec{n}'}\tfrac{1}{\sqrt{q}}\right)_{cd}\right](x)$$
$$- \int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[\sqrt{q}q^{ag}q^{bh}nk_{ab}\right](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\delta^c_{(g}\delta^d_{h)}\delta^{(3)}(x,y)$$
$$+ \int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[\tfrac{1}{2}\sqrt{q}q^{gh}q^{ab}nk_{ab}\right](x)\,[(\pounds_{\vec{n}'}q)_{cd}](y)\delta^c_{(g}\delta^d_{h)}\delta^{(3)}(x,y)$$
$$= \int\limits_\chi d^3x\, \left[nf\left(\pounds_{\vec{n}'}\tfrac{1}{\sqrt{q}}\right)_{cd}\right](x)$$
$$- \int\limits_\chi d^3x\, \left[\sqrt{q}q^{ac}q^{bd}nk_{ab}\right]\left[(\pounds_{\vec{n}'}q)_{cd}\right] + \int\limits_\chi d^3x\, \left[\tfrac{n}{2}\sqrt{q}q^{cd}q^{ab}k_{ab}\right]\left[(\pounds_{\vec{n}'}q)_{cd}\right]$$
$$= \int\limits_\chi d^3x\, \left[nf\left(\pounds_{\vec{n}'}\tfrac{1}{\sqrt{q}}\right)_{cd}\right](x) + \int\limits_\chi d^3x\, [nk_{ab}]\left[(\pounds_{\vec{n}'}q)_{cd}\right]\left(\tfrac{1}{2}\sqrt{q}q^{cd}q^{ab} - \sqrt{q}q^{ac}q^{bd}\right)(x)$$
$$= \int\limits_\chi d^3x\, \left[nf\left(\pounds_{\vec{n}'}\tfrac{1}{\sqrt{q}}\right)_{cd}\right](x) + \int\limits_\chi d^3x\, [nk_{ab}]\left(\pounds_{\vec{n}'}\sqrt{q}q^{ab}\right)(x)$$

5.4. $\int\limits_\chi d^3x \int\limits_\chi d^3y\, \{n(x)c^\varphi(x), n'^b(y)c_b^{\varphi}(y)\}$

$$= \int\limits_\chi d^3x \int\limits_\chi d^3y\, \{n(x)\left[\sum_{J=0}^{3}\left(\frac{(M^{-1})^{JJ}\pi_J\pi_J}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{cd}M_{JJ}\varphi^J_{,c}\varphi^J_{,d}\right)\right](x), n'^b(y)\left[\sum_{I=0}^{3}\pi_I\varphi^I_{,b}\right](y)\}$$
$$= \int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[n\sum_{J=0}^{3}\frac{(M^{-1})^{JJ}}{2\sqrt{q}}\right](x)\left[n'^b\sum_{I=0}^{3}\pi_I\right](y)\{\pi_J(x)\pi_J(x), \varphi^I_{,b}(y)\}$$
$$+ \int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[n\sum_{J=0}^{3}\tfrac{1}{2}\sqrt{q}q^{cd}M_{JJ}\right](x)\left[n'^b\sum_{I=0}^{3}\varphi^I_{,b}\right](y)\{\varphi^J_{,c}(x)\varphi^J_{,d}(x), \pi_I(y)\}$$
$$= -\int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[n\sum_{J=0}^{3}\frac{(M^{-1})^{JJ}}{2\sqrt{q}}\right](x)\left[n'^b\sum_{I=0}^{3}\pi_I\right](y)2\pi_J(x)\delta^I_J\frac{\partial}{\partial y^b}\delta^{(3)}(x,y)$$
$$+ \int\limits_\chi d^3x \int\limits_\chi d^3y\, \left[n\sum_{J=0}^{3}\tfrac{1}{2}\sqrt{q}q^{cd}M_{JJ}\right](x)\left[n'^b\sum_{I=0}^{3}\varphi^I_{,b}\right](y)2\varphi^J_{,c}(x)\delta^J_I\frac{\partial}{\partial x^d}\delta^{(3)}(x,y)$$

$$= -2\int_\chi d^3x \int_\chi d^3y \sum_{J=0}^{3} \left[n\frac{(M^{-1})^{JJ}\pi_J}{2\sqrt{q}}\right](x)\left[n'^b\pi_J\right](y)\frac{\partial}{\partial y^b}\delta^{(3)}(x,y)$$
$$+ 2\int_\chi d^3x \int_\chi d^3y \sum_{J=0}^{3} \left[n\tfrac{1}{2}\sqrt{q}q^{cd}M_{JJ}\varphi^J_{,c}\right](x)\left[n'^b\varphi^J_{,b}\right](y)\frac{\partial}{\partial x^d}\delta^{(3)}(x,y)$$
$$= 2\int_\chi d^3x \sum_{J=0}^{3} \left[n\frac{(M^{-1})^{JJ}\pi_J}{2\sqrt{q}}\right]\left[n'^b\pi_J\right]_{,b} - 2\int_\chi d^3x \sum_{J=0}^{3} \left[n\tfrac{1}{2}\sqrt{q}q^{cd}M_{JJ}\varphi^J_{,c}\right]_{,d}\left[n'^b\varphi^J_{,b}\right]$$
$$= \int_\chi d^3x\, \frac{n}{\sqrt{q}}\frac{\partial f}{\partial \pi_J}\left(\pounds_{\vec{n}'}\pi_J\right)(x) + 2\int_\chi d^3x \sum_{J=0}^{3} \left[n\tfrac{1}{2}\sqrt{q}q^{cd}M_{JJ}\varphi^J_{,c}\right]\left[n'^b_{,d}\varphi^J_{,b} + n'^b\varphi^J_{,db}\right]$$
$$= \int_\chi d^3x\, \frac{n}{\sqrt{q}}\frac{\partial f}{\partial \pi_J}\left(\pounds_{\vec{n}'}\pi_J\right)(x) + \int_\chi d^3x\, n\sqrt{q}q^{cd}\frac{\partial k_{cd}}{\partial \varphi^J_{,d}}\left(\pounds_{\vec{n}'}\varphi^J_{,d}\right)(x)$$
$$= \int_\chi d^3x\, \frac{n}{\sqrt{q}}\left(\pounds_{\vec{n}'}f\right)(x) + \int_\chi d^3x\, n\sqrt{q}q^{cd}\left(\pounds_{\vec{n}'}k\right)_{cd}(x),$$

where we used that π_J is a tensor density of weight one and $\varphi^j_{,a}$ is a covariant vector field of weight 0. For a tensor density ρ of weight 1 the Lie derivative along a vector field n^a is given by $\pounds_{\vec{v}}\rho = \partial_b\left(n^b\rho\right) = \left(n^b\rho\right)_{,b}$ and covariant vector field V_a of weight 0 the Lie derivative along a vector field n^a is given by $\pounds_{\vec{n}}V_a = n^b\partial_b V_a + V_b\partial_a n^b = n^b V_{a,b} + V_b n^b_{,a}$.

Finally, we obtain for term 5.

5. $\int_\chi d^3x \int_\chi d^3y \left\{n(x)c^{\rm tot}(x), n'^b(y)c^{\rm tot}_b(y)\right\}$

$$= \int_\chi d^3x \left[nf\left(\pounds_{\vec{n}'}\frac{1}{\sqrt{q}}\right)_{cd}\right] + \int_\chi d^3x \left[nk_{ab}\right]\left(\pounds_{\vec{n}'}\sqrt{q}q^{ab}\right) + \int_\chi d^3x\, \frac{n}{\sqrt{q}}\left(\pounds_{\vec{n}'}f\right) + \int_\chi d^3x\, n\sqrt{q}q^{cd}\left(\pounds_{\vec{n}'}k\right)_{cd}$$
$$- c^{\rm geo}(\pounds_{\vec{n}'}n)$$
$$= \int_\chi d^3x \left[nf\left(\pounds_{\vec{n}'}\frac{1}{\sqrt{q}}\right)_{cd}\right] + \int_\chi d^3x\, \frac{n}{\sqrt{q}}\left(\pounds_{\vec{n}'}f\right) + \int_\chi d^3x \left[nk_{ab}\right]\left(\pounds_{\vec{n}'}\sqrt{q}q^{ab}\right) + \int_\chi d^3x\, n\sqrt{q}q^{cd}\left(\pounds_{\vec{n}'}k\right)_{cd}$$
$$- c^{\rm geo}(\pounds_{\vec{n}'}n)$$
$$= \int_\chi d^3x\, n\left(\pounds_{\vec{n}'}\frac{f}{\sqrt{q}}\right) + \int_\chi d^3x\, n\left(\pounds_{\vec{n}'}\sqrt{q}q^{ab}k_{ab}\right) - c^{\rm geo}(\pounds_{\vec{n}'}n)$$
$$= \int_\chi d^3x\, n\left(n'^b\frac{f}{\sqrt{q}}\right)_{,b} + \int_\chi d^3x\, n\left(n'^c\sqrt{q}q^{ab}k_{ab}\right)_{,c} - c^{\rm geo}(\pounds_{\vec{n}'}n)$$
$$= -\int_\chi d^3x\, n_{,b}n'^b\frac{f}{\sqrt{q}} - \int_\chi d^3x\, n_{,c}n'^c\sqrt{q}q^{ab}k_{ab} - c^{\rm geo}(\pounds_{\vec{n}'}n)$$
$$= -\int_\chi d^3x\, \left(\pounds_{\vec{n}'}n\right)\frac{f}{\sqrt{q}} - \int_\chi d^3x\, \left(\pounds_{\vec{n}'}n\right)\sqrt{q}q^{ab}k_{ab} - c^{\rm geo}(\pounds_{\vec{n}'}n)$$
$$= -\int_\chi d^3x\, \left(\pounds_{\vec{n}'}n\right)\left(\frac{f}{\sqrt{q}} + \sqrt{q}q^{ab}k_{ab}\right) - c^{\rm geo}(\pounds_{\vec{n}'}n)$$
$$= -\int_\chi d^3x\, \left(\pounds_{\vec{n}'}n\right)c^{\varphi}(x) = -c^{\varphi}(\pounds_{\vec{n}'}n) - c^{\rm geo}(\pounds_{\vec{n}'}n) = -c^{\rm tot}(\pounds_{\vec{n}'}n)$$

E.3.2 Tertiary Constraint $\dot{c}^{\rm tot}(\vec{n})$

II. Calculate

We define the smeared constraint $\vec{c}^{tot}(\vec{n}) := \int\limits_\chi \mathrm{d}^3x\, n^a(x) c_a^{\mathrm{tot}}(x)$ and calculate

$$\begin{aligned}
&\{\vec{c}^{\mathrm{tot}}(\vec{n}), H_{\mathrm{primary}}\} \\
&= \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{tot}(x), \nu(y)z(y)\} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{tot}}(x), \nu^b(y)z_b(y)\} \\
&+ \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{tot}}(x), \sum_{k=1}^{3} \mu_{kk}(y)\Lambda^{kk}(y)\} \\
&+ \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{tot}}(x), n'(y)c^{\mathrm{tot}}(y)\} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{tot}}(x), n'^b(y)c_b^{\mathrm{tot}}(y)\}.
\end{aligned} \tag{866}$$

1. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{tot}}(x), \nu(y)z(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \underbrace{\{n^a(x)c_a^{\mathrm{geo}}(x), \nu(y)p(y)\}}_{=0} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \underbrace{\{n^a(x)c_a^{\varphi}(x), \nu(y)p(y), \}}_{=0} = 0$

2. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{tot}}(x), \nu^b(y)z_b(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{geo}}(x), \nu^b(y)p_b(y)\} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\varphi}(x), \nu^b(y)p_b(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \nu^b(y)c_a^{\mathrm{geo}}(x) \underbrace{\{n^a(x), p_b(y)\}}_{\delta_b^a \delta^{(3)}(x,y)} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \nu^b(y)c_a^{\varphi}(x) \underbrace{\{n^a(x), p_b(y)\}}_{\delta_b^a \delta^{(3)}(x,y)}$
$= \int\limits_\chi \mathrm{d}^3x\, \nu^a(x)c_a^{\mathrm{tot}}(x) = \vec{c}^{\mathrm{tot}}(\vec{\nu})$

3. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{tot}}(x), \mu_{kk}(y)\Pi^{kk}(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \underbrace{\{n^a(x)c_a^{\mathrm{geo}}(x), \mu_{kk}(y)\Pi^{kk}(y)\}}_{=0} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \underbrace{\{n^a(x)c_a^{\varphi}(x), \mu_{kk}(y)\Pi^{kk}(y)\}}_{=0} = 0$

4. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{tot}}(x), n'(y)c^{\mathrm{tot}}(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{geo}}(x), n'(y)c^{\mathrm{tot}}(y)\} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\varphi}(x), n'(y)c^{\mathrm{tot}}(y)\}$
$= \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{geo}}(x), n'(y)c^{\mathrm{geo}}(y)\} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{geo}}(x), n'(y)c^{\varphi}(y)\}$
$+ \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\varphi}(x), n'(y)c^{\mathrm{geo}}(y)\} + \int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\varphi}(x), n'(y)c^{\varphi}(y)\}$

 4.1. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{geo}}(x), n'(y)c^{\mathrm{geo}}(y)\} = \{\vec{c}^{\mathrm{geo}}(\vec{n}), c^{\mathrm{geo}}(n')\} = c^{\mathrm{geo}}(\pounds_{\vec{n}} n')$

 4.2. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\mathrm{geo}}(x), n'(y)c^{\varphi}(y)\}$
 $= -\int\limits_\chi \mathrm{d}^3x \left[n' f \left(\pounds_{\vec{n}} \frac{1}{\sqrt{q}}\right)_{cd}\right](x) - \int\limits_\chi \mathrm{d}^3x\, [n' k_{ab}] \left(\pounds_{\vec{n}} \sqrt{q} q^{ab}\right)(x)$

 4.3. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\varphi}(x), n'(y)c^{\mathrm{geo}}(y)\} = 0$

 4.4. $\int\limits_\chi \mathrm{d}^3x \int\limits_\chi \mathrm{d}^3y\, \{n^a(x)c_a^{\varphi}(x), n'(y)c^{\varphi}(y)\}$
 $= -\int\limits_\chi \mathrm{d}^3x\, \frac{n'}{\sqrt{q}} \left(\pounds_{\vec{n}} f\right)(x) - \int\limits_\chi \mathrm{d}^3x\, n' \sqrt{q} q^{cd} \left(\pounds_{\vec{n}} k\right)_{cd}(x)$

5. $\int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\text{tot}}(x), n'^b(y)c_b^{\text{tot}}(y)\}$
$= \int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\text{geo}}(x), n'^b(y)c_b^{\text{tot}}(y)\} + \int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\text{tot}}(y)\}$
$= \int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\text{geo}}(x), n'^b(y)c_b^{\text{geo}}(y)\} + \int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\text{geo}}(x), n'^b(y)c_b^{\varphi}(y)\}$
$+ \int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\text{geo}}(y)\} + \int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\varphi}(y)\}$

5.1. $\int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\text{geo}}(x), n'^b(y)c_b^{\text{geo}}(y)\} = \{\vec{c}^{\text{geo}}(\vec{n}), \vec{c}^{\text{geo}}(\vec{n'})\} = \vec{c}^{\text{geo}}(\pounds_{\vec{n}}\vec{n}')$

5.2. $\int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\text{geo}}(x), n'^b(y)c_b^{\varphi}(y)\} = 0$

5.3. $\int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\text{geo}}(y)\} = 0$

5.4. $\int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\varphi}(x), n'^b(y)c_b^{\varphi}(y)\}$

$$= \int\limits_\chi d^3x \int\limits_\chi d^3y\, n^a(x)n'^b(y)\{\left[\sum_{J=0}^3 \pi_J\varphi^J_{,a}\right](x), \left[\sum_{I=0}^3 \pi_I\varphi^I_{,b}\right](y)\}$$
$$= \int\limits_\chi d^3x \int\limits_\chi d^3y\, n^a(x)n'^b(y) \sum_{J=0}^3\sum_{I=0}^3 \Big(\pi_J(x)\varphi^I_{,b}(y)\{\varphi^J_{,a}(x), \pi_I(y)\} + \varphi^J_{,a}(x)\pi_I(y)\{\pi_J(x), \varphi^I_{,b}(y)\}\Big)$$
$$= \int\limits_\chi d^3x \int\limits_\chi d^3y\, n^a(x)n'^b(y) \sum_{J=0}^3\sum_{I=0}^3 \Big(\pi_J(x)\varphi^I_{,b}(y)\delta^J_I \tfrac{\partial}{\partial x^a}\delta^{(3)}(x,y) - \varphi^J_{,a}(x)\pi_I(y)\delta^I_J\tfrac{\partial}{\partial y^b}\delta^{(3)}(x,y)\Big)$$
$$= \int\limits_\chi d^3x \sum_{J=0}^3 \Big(-\left[n^a\pi_J\right]_{,a} n'^b\varphi^J_{,b} + n^a\varphi^J_{,a}\left[n'^b\pi_J\right]_{,b}\Big)$$
$$= \int\limits_\chi d^3x \sum_{J=0}^3 \Big(-n^a_{,a}n'^b\varphi^J_{,b}\pi_J - n^an'^b\varphi^J_{,b}\pi_{J,a} + n^an'^b_{,b}\varphi^J_{,a}\pi_J + n^an'^b\varphi^J_{,a}\pi_{J,b}\Big)$$
$$\overset{\text{PI}}{=} \int\limits_\chi d^3x \sum_{J=0}^3 \Big(-n^a_{,a}n'^b\varphi^J_{,b}\pi_J + \left[n^an'^b\varphi^J_{,b}\right]_{,a}\pi_J + n^an'^b_{,b}\varphi^J_{,a}\pi_J - \left[n^an'^b\varphi^J_{,a}\right]_{,b}\pi_J\Big)$$
$$= \int\limits_\chi d^3x \sum_{J=0}^3 \Big(-n^a_{,a}n'^b\varphi^J_{,b}\pi_J + n^a_{,a}n'^b\varphi^J_{,b}\pi_J + n^an'^b_{,a}\varphi^J_{,b}\pi_J + n^an'^b\varphi^J_{,ba}\pi_J$$
$$+n^an'^b_{,b}\varphi^J_{,a}\pi_J - n^a_{,b}n'^b\varphi^J_{,a}\pi_J - n^an'^b_{,b}\varphi^J_{,a}\pi_J - n^an'^b\varphi^J_{,ba}\pi_J\Big)$$
$$= \int\limits_\chi d^3x \sum_{J=0}^3 \Big(n^an'^b_{,a}\varphi^J_{,b}\pi_J - n^a_{,b}n'^b\varphi^J_{,a}\pi_J\Big)$$
$$= \int\limits_\chi d^3x \Big(n^bn'^a_{,b} - n'^bn^a_{,b}\Big)c^\varphi_a = \vec{c}^\varphi(\pounds_{\vec{n}}\vec{n}')$$

The addition of 4.3 and 4.4 leads to $c^\varphi(\pounds_{\vec{n}}n')$. In summary we obtain for term 4. and 5.

4. $\int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\text{tot}}(x), n'(y)c^{\text{tot}}(y)\} = c^\varphi(\pounds_{\vec{n}}n') + c^{\text{geo}}(\pounds_{\vec{n}}n') = c^{\text{tot}}(\pounds_{\vec{n}}n')$.

5. $\int\limits_\chi d^3x \int\limits_\chi d^3y \{n^a(x)c_a^{\text{tot}}(x), n'^b(y)c_b^{\text{tot}}(y)\} = \vec{c}^{\text{geo}}(\pounds_{\vec{n}}\vec{n}') + \vec{c}^\varphi(\pounds_{\vec{n}}\vec{n}') = \vec{c}^{\text{tot}}(\pounds_{\vec{n}}\vec{n}')$

F Calculation of β_{jj}

Large parts of this section have been published in [130]. The expression for β_{jj} reads

$$
\begin{aligned}
\beta_{jj}(x) &= -\int\limits_{\chi} \mathrm{d}^3y\sqrt{q}\frac{(M_{jj})^3}{n\pi_j^2}\{c^{\mathrm{tot}}(x), c^{jj}(y)\} \\
&= -\int\limits_{\chi} \mathrm{d}^3y\sqrt{q}\frac{(M_{jj})^3}{n\pi_j^2}\left(\{c^{\mathrm{geo}}(x), c^{jj}(y)\} + \{c^{\phi}(x), c^{jj}(y)\}\right) \\
&= -\sqrt{q}\frac{(M_{jj})^3}{n\pi_j^2}\Bigg(-\frac{1}{2\sqrt{q}}c^{jj}\left(p^{ab}q_{ab}\right) - n\varphi^j_{,a}\varphi^j_{,b}\,p^{ab} \\
&\quad - \left[\frac{(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right]\left[n\sqrt{q}q^{ab}\varphi^j_{,b}\right]_{,a} - \left[\sqrt{q}M_{jj}q^{ab}\varphi^j_{,b}\right]_{,a}\left[n\frac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right]\Bigg) \\
&= \frac{(M_{jj})^3}{2n\pi_j^2}c^{jj}\left(p^{ab}q_{ab}\right) + \sqrt{q}\frac{(M_{jj})^3}{\pi_j^2}\varphi^j_{,a}\varphi^j_{,b}\,p^{ab} + \frac{(M_{jj})^2}{n\pi_j}\left[n\sqrt{q}q^{ab}\varphi^j_{,b}\right]_{,a} + \frac{M_{jj}}{\pi_j}\left[\sqrt{q}M_{jj}q^{ab}\varphi^j_{,b}\right]_{,a},
\end{aligned}
$$

where we make use of the calculation of the Poisson bracktes. First we calculate

$$
\begin{aligned}
\int_\chi d^3y\{\kappa c^{\mathrm{geo}}(x), c^{jj}(y)\} =& \int_\chi d^3y\Big\{\left[\frac{1}{\sqrt{q}}\left(q_{ac}qbd-\frac{1}{2}q_{ab}q_{cd}\right)p^{ab}p^{cd}-\sqrt{q}R^{(3)}+2\sqrt{q}\Lambda\right](x),\\
&\left[\frac{n}{2}\left[\sum_{k=1}^{3}\frac{(M^{-1})^{jk}(M^{-1})^{jk}\pi_k\pi_k}{\sqrt{q}}-\sqrt{q}q^{ef}\varphi^j_{,e}\varphi^j_{,f}\right]\right](y)\Big\}\\
\overset{M^{jk}\neq 0 \text{ for } j=k}{=}& \int_\chi d^3y\left[\frac{1}{\sqrt{q}}\left(q_{ac}qbd-\frac{1}{2}q_{ab}q_{cd}\right)\right](x)\left[\frac{n}{2}(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j\right](y)\\
&\{p^{ab}(x)p^{cd}(x),\frac{1}{\sqrt{q}}(y)\}\\
&-\int_\chi d^3y\left[\frac{1}{\sqrt{q}}\left(q_{ac}qbd-\frac{1}{2}q_{ab}q_{cd}\right)\right](x)\left[\frac{n}{2}\varphi^j_{,e}\varphi^j_{,f}\right](y)\\
&\{p^{ab}(x)p^{cd}(x),\sqrt{q}(y)q^{ef}(y)\}\\
=& \int_\chi d^3y\left[\frac{1}{\sqrt{q}}\left(q_{ac}qbd-\frac{1}{2}q_{ab}q_{cd}\right)\right](x)\left[\frac{n}{2}(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j\right](y)\\
&\left(p^{ab}(x)\{p^{cd}(x),\frac{1}{\sqrt{q}}(y)\}+p^{cd}(x)\{p^{ab}(x),\frac{1}{\sqrt{q}}(y)\}\right)\\
&-\int_\chi d^3y\left[\frac{1}{\sqrt{q}}\left(q_{ac}qbd-\frac{1}{2}q_{ab}q_{cd}\right)\right](x)\left[\frac{n}{2}\varphi^j_{,e}\varphi^j_{,f}\right](y)\\
&\big(p^{ab}(x)q^{ef}(y)\{p^{cd}(x),\sqrt{q}(y)\}+p^{ab}(x)\sqrt{q}(y)\{p^{cd}(x),q^{ef}(y)\}\\
&+p^{cd}(x)q^{ef}(y)\{p^{ab}(x),\sqrt{q}(y)\}+p^{cd}(x)\sqrt{q}(y)\{p^{ab}(x),q^{ef}(y)\}\big)\\
=& \int_\chi d^3y\left[\frac{1}{\sqrt{q}}\left(q_{ac}qbd-\frac{1}{2}q_{ab}q_{cd}\right)\right](x)\left[\frac{n}{2}(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j\right](y)\\
&\left(p^{ab}(x)(-\frac{1}{2\sqrt{q}}q^{ef})(y)(-\kappa\delta^c_{(e}\delta^d_{f)})\delta^{(3)}(x,y)+p^{cd}(x)(-\frac{1}{2\sqrt{q}}q^{ef})(y)(-\kappa\delta^a_{(e}\delta^b_{f)})\delta^{(3)}(x,y)\right)\\
&-\int_\chi d^3y\left[\frac{1}{\sqrt{q}}\left(q_{ac}qbd-\frac{1}{2}q_{ab}q_{cd}\right)\right](x)\left[\frac{n}{2}\varphi^j_{,e}\varphi^j_{,f}\right](y)\\
&\Big(p^{ab}(x)(\frac{1}{2}\sqrt{q}q^{ef}q^{gh})(y)(-\kappa\delta^c_{(g}\delta^d_{h)})\delta^{(3)}(x,y)+p^{cd}(x)(\frac{1}{2}\sqrt{q}q^{ef}q^{gh})(y)(-\kappa\delta^a_{(g}\delta^b_{h)})\delta^{(3)}(x,y)\\
&+p^{ab}(x)(-\sqrt{q}q^{ge}q^{hf})(y)(-\kappa\delta^c_{(g}\delta^d_{h)})\delta^{(3)}(x,y)+p^{cd}(x)(-\sqrt{q}q^{ge}q^{hf})(y)(-\kappa\delta^a_{(g}\delta^b_{h)})\delta^{(3)}(x,y)\Big)\\
\overset{q^{ab}\equiv q^{ba}}{=}& \kappa\frac{1}{2\sqrt{q}}\left[\frac{1}{\sqrt{q}}\left(q_{ac}q_{bd}-\frac{1}{2}q_{ab}q_{cd}\right)\right]\left[\frac{n}{2}(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j\right]\left(p^{ab}q^{cd}+p^{cd}q^{ab}\right)\\
&+\kappa\frac{1}{2}\sqrt{q}\left[\frac{1}{\sqrt{q}}\left(q_{ac}q_{bd}-\frac{1}{2}q_{ab}q_{cd}\right)\right]\left[\frac{n}{2}\varphi^j_{,e}\varphi^j_{,f}\right]\left(p^{ab}q^{ef}q^{cd}+p^{cd}q^{ef}q^{ab}\right)\\
&-\kappa\sqrt{q}\left[\frac{1}{\sqrt{q}}\left(q_{ac}q_{bd}-\frac{1}{2}q_{ab}q_{cd}\right)\right]\left[\frac{n}{2}\varphi^j_{,e}\varphi^j_{,f}\right]\left(p^{ab}q^{ce}q^{df}+p^{cd}q^{ae}q^{bf}\right)\\
=& \kappa\frac{1}{2\sqrt{q}}\frac{1}{\sqrt{q}}\left[\frac{n}{2}(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j\right]\left(-p^{ab}q_{ab}\right)\\
&+\kappa\sqrt{q}\frac{1}{\sqrt{q}}\left[\frac{n}{2}\varphi^j_{,e}\varphi^j_{,f}\right]\left(-\frac{1}{2}p^{ab}q_{ab}q^{ef}\right)+\kappa\sqrt{q}\frac{1}{\sqrt{q}}\left[\frac{n}{2}\varphi^j_{,e}\varphi^j_{,f}\right]\left(-2p^{ef}+p^{ab}q_{ab}q^{ef}\right)\\
=& -\kappa\frac{1}{2\sqrt{q}}\frac{n}{2}\left[\frac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j\pi_j}{\sqrt{q}}+\sqrt{q}q^{ef}\varphi^j_{,e}\varphi^j_{,f}\right]\left(p^{ab}q_{ab}\right)-\kappa n\varphi^j_{,a}\varphi^j_{,b}\,p^{ab}\\
=& -\kappa\frac{1}{2\sqrt{q}}c^{jj}\left(p^{ab}q_{ab}\right)-\kappa n\varphi^j_{,a}\varphi^j_{,b}\,p^{ab}.
\end{aligned}
$$

Next we calculate

$$
\begin{aligned}
\int_{\chi} d^3y\{c^{\varphi}(x), c^{jj}(y)\} =& \int_{\chi} d^3y\Big\{ \left[\frac{\pi_0^2}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}q^{ab}\varphi^0_{,a}\varphi^0_{,b} + \sum_{\ell=1}^{3}\left(\frac{(M^{-1})^{\ell\ell}\pi_\ell\pi_\ell}{2\sqrt{q}} + \frac{1}{2}\sqrt{q}M_{\ell\ell}q^{ab}\varphi^{\ell}_{,a}\varphi^{\ell}_{,b}\right)\right](x), \\
& \left[\frac{n}{2}\left[\sum_{k=1}^{3}\frac{(M^{-1})^{jk}(M^{-1})^{jk}\pi_k\pi_k}{\sqrt{q}} - \sqrt{q}q^{cd}\varphi^j_{,c}\varphi^j_{,d}\right]\right](y)\Big\} \\
=& -\int_{\chi} d^3y\Big\{\left[\sum_{\ell=1}^{3}\frac{(M^{-1})^{\ell\ell}\pi_\ell\pi_\ell}{2\sqrt{q}}\right](x), \left[\frac{n}{2}\sqrt{q}q^{cd}\varphi^j_{,c}\varphi^j_{,d}\right](y)\Big\} \\
& + \int_{\chi} d^3y\Big\{\left[\sum_{\ell=1}^{3}\frac{1}{2}\sqrt{q}M_{\ell\ell}q^{ab}\varphi^{\ell}_{,a}\varphi^{\ell}_{,b}\right](x), \left[\frac{n}{2}\sum_{k=1}^{3}\frac{(M^{-1})^{jk}(M^{-1})^{jk}\pi_k\pi_k}{\sqrt{q}}\right](y)\Big\} \\
=& -\int_{\chi} d^3y\left[\sum_{\ell=1}^{3}\frac{(M^{-1})^{\ell\ell}}{2\sqrt{q}}\right](x), \left[\frac{n}{2}\sqrt{q}q^{cd}\right](y)\{\pi_\ell(x)\pi_\ell(x), \varphi^j_{,c}(y)\varphi^j_{,d}(y)\} \\
& + \int_{\chi} d^3y\left[\sum_{\ell=1}^{3}\frac{1}{2}\sqrt{q}M_{\ell\ell}q^{ab}\right](x), \left[\frac{n}{2}\sum_{k=1}^{3}\frac{(M^{-1})^{jk}(M^{-1})^{jk}}{\sqrt{q}}\right](y)\{\varphi^{\ell}_{,a}(x)\varphi^{\ell}_{,b}(x), \pi_k(y)\pi_k(y)\} \\
\stackrel{q^{ab}=q^{ba}}{=}& -\int_{\chi} d^3y\left[\sum_{\ell=1}^{3}\frac{(M^{-1})^{\ell\ell}}{2\sqrt{q}}\right](x), \left[\frac{n}{2}\sqrt{q}q^{cd}\right](y)\,4\pi_\ell(x)\varphi^j_{,d}(y)\{\pi_\ell(x), \varphi^j_{,c}(y)\} \\
& + \int_{\chi} d^3y\left[\sum_{\ell=1}^{3}\frac{1}{2}\sqrt{q}M_{\ell\ell}q^{ab}\right](x), \left[\frac{n}{2}\sum_{k=1}^{3}\frac{(M^{-1})^{jk}(M^{-1})^{jk}}{\sqrt{q}}\right](y)\,4\varphi^{\ell}_{,b}(x)\pi_k(y)\{\varphi^{\ell}_{,a}(x), \pi_k(y)\} \\
=& -\int_{\chi} d^3y\left[\sum_{\ell=1}^{3}\frac{(M^{-1})^{\ell\ell}}{\sqrt{q}}\right](x)\left[n\sqrt{q}q^{cd}\right](y)\,\pi_\ell(x)\varphi^j_{,d}(y)\left(-\delta^j_\ell\frac{\partial}{\partial y^c}\delta^{(3)}(x,y)\right) \\
& + \int_{\chi} d^3y\left[\sum_{\ell=1}^{3}\sqrt{q}M_{\ell\ell}q^{ab}\right](x)\left[n\sum_{k=1}^{3}\frac{(M^{-1})^{jk}(M^{-1})^{jk}}{\sqrt{q}}\right](y)\,\varphi^{\ell}_{,b}(x)\pi_k(y)\left(\delta^{\ell}_k\frac{\partial}{\partial x^c}\delta^{(3)}(x,y)\right) \\
=& \int_{\chi} d^3y\left[\frac{(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right](x)\left[n\sqrt{q}q^{cd}\varphi^j_{,d}\right](y)\left(\frac{\partial}{\partial y^c}\delta^{(3)}(x,y)\right) \\
& + \int_{\chi} d^3y\left[\sum_{k=1}^{3}\sqrt{q}M_{kk}q^{ab}\varphi^k_{,b}\right](x)\left[n\frac{(M^{-1})^{jk}(M^{-1})^{jk}\pi_k}{\sqrt{q}}\right](y)\left(\frac{\partial}{\partial x^c}\delta^{(3)}(x,y)\right) \\
=& -\left[\frac{(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right]\left[n\sqrt{q}q^{ab}\varphi^j_{,b}\right]_{,a} - \left[\sum_{k=1}^{3}\sqrt{q}M_{kk}q^{ab}\varphi^k_{,b}\right]_{,a}\left[n\frac{(M^{-1})^{jk}(M^{-1})^{jk}\pi_k}{\sqrt{q}}\right] \\
\stackrel{M^{jk}\neq 0 \text{ for } j=k}{=}& -\left[\frac{(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right]\left[n\sqrt{q}q^{ab}\varphi^j_{,b}\right]_{,a} - \left[\sqrt{q}M_{jj}q^{ab}\varphi^j_{,b}\right]_{,a}\left[n\frac{(M^{-1})^{jj}(M^{-1})^{jj}\pi_j}{\sqrt{q}}\right].
\end{aligned}
$$

The rather lengthy but straightforward calculation presented above shows that

$$\begin{aligned}\beta_{jj}(x) =& \frac{1}{2}\frac{(M_{jj})^3}{n\pi_j^2} q_{ab}p^{ab}c^{jj}(x) + \sqrt{q}\varphi^j_{,a}\varphi^j_{,b}p^{ab}\frac{(M_{jj})^3}{\pi_j^2}(x) \\ &+ \frac{(M_{jj})^2}{n\pi_j}\left(n\sqrt{q}q^{ab}\varphi^j_{,b}\right)_{,a}(x) + \frac{(M_{jj})}{\pi_j}\left(M_{jj}\sqrt{q}q^{ab}\varphi^j_{,b}\right)_{,a}(x).\end{aligned}$$

G Lemmata from the AQG III Article

We recall here two lemmata from [4], since they are used throughout the calculation for several times .

Lemma 2.1. *For each $k \geq 0$ there exists $0 < \beta_k < \infty$ such that*

$$f_{2k+1}(t) - \beta_k t^{2k+2} \leq f(t) \leq f_{2k+1}(t),$$

where $f_k(t)$ denotes the partial Taylor series of $f(t) = (1+t)^q$, $0 < q \leq 1/4$ up to order t^k.

Lemma 2.3. *Let $B_- \leq B \leq B_+$ be self-adjoint operators and set $\bar{B} := [B_+ + B_-/2]$, $\Delta B := [B_+ - B_-/4]$. Then for any states ψ_1, ψ_2 in the common domain of all three operators we have*

$$|\Re(\langle\psi_1, [B-\bar{B}]\psi_2\rangle)|, \quad |\Im(\langle\psi_1, [B-\bar{B}]\psi_2\rangle)| \leq \langle\psi_1, [\Delta B]\psi_1\rangle + \langle\psi_2, [\Delta B]\psi_2\rangle.$$

H Additional Calculations Semiclassical States

H.1 Coherent States for SUSY Potentials

The method we will present here was first applied to special problems in supersymmetry, but as for example Nieto [34] and Molski [174] showed that it proved to be useful to construct coherent states for a special class of potentials $V(q)$, so-called supersymmetric potentials, which have a certain functional form we will display below. In [34] used this method to construct coherent states for the double well potential and linear (gravitational) potential.

For convenience we will now absorb all prefactors in the new variable x so that the Schrödinger equation in the position representation has the form

$$H = -\partial_x^2 + V(x). \tag{867}$$

The statement of [34] is that in analogy to the annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$ one can define $\hat{A}$ and $\hat{A}^\dagger$ for more general potentials, if $V(x)$ is a so-called supersymmetric potential. A potential is called ***supersymmetric*** if it has the form

$$V(x) = [W'(x)]^2 - W''(x) \tag{868}$$

for an at least two times with respect to x differentiable function $W(x)$. With the knowledge of $W(x)$ we can define $\hat{A}$ and $\hat{A}^\dagger$ in the position representation to be

$$A := \partial_x + W'(x), \;\; A^\dagger := -\partial_x + W'(x), \tag{869}$$

and rewrite H as $H = A^\dagger A$. The normalized ground state function is according to [34] is given by

$$\psi_0(x) = N_0 \exp\left[-W(x)\right] \tag{870}$$

As a generalization of the coherent states as annihilation operator eigenstates we demand

$$A(x)\psi_\alpha(x) = \alpha\psi_\alpha(x)$$

and find the coherent states ψ_α to be

$$\psi_\alpha(x) = N_\alpha \exp\left[\alpha x - W(x)\right] = \rho(x)\exp\left[\alpha x\right]\psi_0(x), \tag{871}$$

where $N_\alpha = \rho(x)N_0$ is a normalization (phase) factor and $\alpha \in \mathbb{C}$.

Vice versa we can make an ansatz for $W(x)$ and calculate the possible potentials which can be handled. Consider for example the second order polynomial

$$W(x) = c_2x^2 + c_1x + c_0, \tag{872}$$

where $c_k \in \mathbb{R}, k \in \mathbb{N}_0$ are constants, which gives rise to the supersymmetric potential

$$V(x) = 4c_2^2x^2 + 4c_1c_2x + c_1^2 - 2c_2$$

or analogous higher order polynomials and their corresponding supersymmetric potentials like

$$\begin{aligned}
W(x) &= c_3x^3 + c_2x^2 + c_1x + c_0,\\
V(x) &= 9c_3^2x^4 + 12c_2c_3x^3 + \left(6c_1c_3 + 4c_2^2\right)x^2 + 4c_1c_2x + c_1^2 - \left[2c_2 + 6c_3x\right].
\end{aligned}$$

We are interested in the algebra of the new A, $A^\dagger$ and H, so we will in the following calculate the commutators in the position representation by applying them to a test function $\psi(x)$,

$$\left[A, A\right]\psi(x) = \left[A^\dagger, A^\dagger\right]\psi(x) = \left[H, H\right]\psi(x) = 0. \tag{873}$$

and

$$\begin{aligned}
&\left[A^\dagger, A\right]\psi(x) \\
&= \left(-\partial_x + W'(x)\right)\left(\partial_x + W'(x)\right)\psi(x) - \left(\partial_x + W'(x)\right)\left(-\partial_x + W'(x)\right)\psi(x)\\
&= \left(-\partial_x + W'(x)\right)\left(\psi'(x) + W'(x)\psi(x)\right) - \left(\partial_x + W'(x)\right)\left(-\psi'(x) + W'(x)\psi(x)\right)\\
&= -\psi''(x) - W''(x)\psi(x) - W'(x)\psi'(x) + W'(x)\psi'(x) + \left[W'(x)\right]^2\psi(x)\\
&+ \psi''(x) - W''(x)\psi(x) - W'(x)\psi'(x) + W'(x)\psi'(x) - \left[W'(x)\right]^2\psi(x)\\
&= -2W''(x)\psi(x).
\end{aligned} \tag{874}$$

With the help of the commutators calculated above, we can further derive the commutators

$$\begin{aligned}
\left[H, A\right]\psi(x) &= A^\dagger\left[A, A\right]\psi(x) + \left[A^\dagger, A\right]A\psi(x) = -2W''(x)A\psi(x),\\
\left[H, A^\dagger\right]\psi(x) &= A^\dagger\left[A, A^\dagger\right]\psi(x) + \left[A^\dagger, A^\dagger\right]A\psi(x) = 2A^\dagger W''(x)\psi(x).
\end{aligned} \tag{875}$$

Then we count $W''(x)$ as a new generator of the algebra and go on with the calculation of the commutators to get to know more of the algebraic structure

$$\begin{aligned}
&\left[W''(x), A\right]\psi(x) \\
&= W''(x)\left(\partial_x + W'(x)\right)\psi(x) - \left(\partial_x + W'(x)\right)W''(x)\psi(x)\\
&= W''(x)\left(\psi'(x) + W'(x)\psi(x)\right) - W'''(x)\psi(x) - W''(x)\psi'(x) - W'(x)W''(x)\psi(x)\\
&= W''(x)\psi'(x) + W''(x)W'(x)\psi(x) - W'''(x)\psi(x) - W''(x)\psi'(x) - W''(x)W'(x)\psi(x)\\
&= -W'''(x)\psi(x),
\end{aligned} \tag{876}$$

since $[W''(x), W'(x)] = 0$ and analogous for

$$\begin{aligned}
&\left[W^{(n)}(x), A\right] \psi(x) = -W^{(n+1)}(x)\psi(x), \qquad (877)\\
&\left[W^{(n)}(x), A^\dagger\right] \psi(x) = W^{(n+1)}(x)\psi(x),\\
&\left[W^{(n)}(x), H\right] \psi(x) = \left[W^{(n)}(x), A^\dagger A\right] \psi(x) = \left(A^\dagger W^{(n+1)}(x) + W^{(n+1)}(x)A\right) \psi(x)
\end{aligned}$$

with $n \in \mathbb{N}_0$. For a polynomial of degree n, the $n+1$ derivative and every higher derivative is going to vanish $W^{(n+1)} = W^{(n+2)} = \ldots = 0$. Therefore, the algebra will be closed. In our example for $n = 2$, we have

$$W(x) = c_2x^2 + c_1x + c_0, \quad W''(x) = 2c_2, \quad W^{(n)} = 0 \quad n \geq 2, \qquad (878)$$

therefore the commutators become

$$\left[A^\dagger, A\right] \psi(x) = -4c_2\psi(x), \quad [H, A]\, \psi(x) = -4c_2A\psi(x), \quad \left[H, A^\dagger\right] \psi(x) = 4c_2A^\dagger\psi(x).$$

This method seems promising for certain types of polynomial potentials. Despite that, one needs to check whether the so constructed states really satisfy all characteristics a coherent state should have.

H.2 Symmetries of Differential Equations- Free Particle

We apply the method expalined in section 20.2.1 to the case of a free particle in one dimension. The Lagrangian for the free particle with mass $m \neq 0$ is

$$L(t, q(t), \dot{q}(t)) = \frac{m}{2}\dot{q}^2, \qquad (879)$$

where a dot denotes the derivative with respect to the time parameter t An ansatz for its first integral is given by

$$\varphi = \frac{1}{2}K_{11}\dot{q}^2 + K_1\dot{q} + K, \qquad (880)$$

where K_{11}, K_1 and K are functions of t and $q(t)$. The equation of motion for the free particle reads

$$\ddot{q} = 0. \qquad (881)$$

We calculate the total time derivative of φ and we try to find the conditions for which it becomes zero:

$$\begin{aligned}
0 \stackrel{!}{=} \frac{\mathrm{d}}{\mathrm{d}t}\varphi =& \frac{1}{2}\left(K_{11,q}\dot{q} + K_{11,t}\right)\dot{q}^2 + \frac{1}{2}K_{11}2\dot{q}\ddot{q} \qquad (882)\\
&\left(K_{1,q}\dot{q} + K_{1,t}\right)\dot{q} + K_1\ddot{q}\\
&+ K_{,q}\dot{q} + K_{,t}\\
\stackrel{\ddot{q}=0}{=}& \frac{1}{2}K_{11,q}\dot{q}^3 + \left(\frac{1}{2}K_{11,t} + K_{1,q}\right)\dot{q}^2\\
&+ \left(K_{1,t} + K_{,q}\right)\dot{q} + K_{,t},
\end{aligned}$$

where a comma followed by a letter means a partial derivative with respect to the correspondig variable. Therefore, for the third order term we obtain

$$\frac{1}{2}K_{11,q} = 0 \Rightarrow K_{11} = a(t). \tag{883}$$

The second order terms lead to

$$\begin{aligned}
&\frac{1}{2}K_{11,t} + K_{1,q} = 0 \Leftrightarrow K_{1,q} = -\frac{1}{2}K_{11,t} = -\frac{1}{2}a_{,t} \\
&\Rightarrow K_1 = -\frac{1}{2}a_{,t}q + b(t)
\end{aligned} \tag{884}$$

and

$$K_{1,t} = -\frac{1}{2}a_{,tt}q - \frac{1}{2}a_{,t}\dot{q} + b_{,t}. \tag{885}$$

We insert the results obtained so far again in the first integral condition to determine the function K

$$\begin{aligned}
0 \stackrel{!}{=} \frac{\mathrm{d}}{\mathrm{d}t}\varphi =& K_{1,t}\dot{q} + K_{,q}\dot{q} + K_{,t} \\
=& -\frac{1}{2}a_{,tt}q\dot{q} - \frac{1}{2}a_{,t}\dot{q}^2 + b_{,t}\dot{q} + K_{,q}\dot{q} + K_{,t}.
\end{aligned} \tag{886}$$

From this we can conclude that $a_{,tt}$ and a_t have to vanish i.e. $a_{,tt} = a_{,t} = 0$ in oder to get rid of the mixed terms and second order terms which is the case for $a_{,t} = const. := c_1$ being a constant. Now we are left with

$$b_{,t} + K_{,x} = 0 \Rightarrow K = -b_{,t}q + c(t) \tag{887}$$

and

$$K_{,t} = -b_{,tt}q + -b_{,t}\dot{q} + c_{,t} = 0 \tag{888}$$

which is only satisfied for $b_{,t} = b_{,tt} = 0$ and $c_{,t} = 0$ which means that $b(t) = const. =: c_2$ and $c(t) = const =: c_3$.The first integral is finally given by

$$\varphi = \frac{1}{2}c_1\dot{q}^2 + c_2\dot{q} + c_3. \tag{889}$$

Check

$$\frac{\mathrm{d}}{\mathrm{d}t}\varphi = c_1\dot{q}\ddot{q} + c_2\ddot{q} = 0 \tag{890}$$

using the equation of motion $\ddot{q} = 0$.

For the free particle we obtain

$$\begin{aligned}
&\frac{\partial^2 L}{\partial\dot{q}\partial\dot{q}}\left(\eta - \dot{q}\xi\right) = -\frac{\partial\varphi}{\partial\dot{q}} \\
&\Leftrightarrow m\left(\eta - \dot{q}\xi\right) = -c_1\dot{q} - c_2 \\
&\Rightarrow \xi = \frac{c_1}{m}, \quad \eta = -\frac{c_2}{m}
\end{aligned} \tag{891}$$

for arbitray constraints c_1, $c_2 \in \mathbb{R}$. The generator of the Problem is given by

$$X = \frac{c_1}{m}\frac{\partial}{\partial t} - \frac{c_2}{m}\frac{\partial}{\partial q} \tag{892}$$

or we can also chose for example $c_1 = 0$, $c_2 = 1$ and $c_1 = 1$, $c_2 = 0$ and write down one generator for each parameter, that is

$$X_1 = -\frac{1}{m}\frac{\partial}{\partial q}, \quad X_2 = \frac{1}{m}\frac{\partial}{\partial t}. \tag{893}$$

Assuming that the partial derivative applied to a smooth function can be interchanged, their commutator vanishes

$$[X_1, X_2] = 0. \tag{894}$$

We see that this is a special case of the generator for the free particle mentioned in [54], when t and q have constant values.

I Proof Coherence Breaking

In the upcoming we reproduce a proof given in [61] with additional explainations in order to gain a better understanding of what happens during coherence breaking. Following [61] let $W(t)$ be a time-dependent function $W(t)$ of compact support which when added to the Hamiltonian causes the breaking of the coherence of the, with respect to the original Hamiltonian, coherent states. It is assumed that $W(t)$ is a small perturbation in comparison to the Hamiltonian H. In [61] it is stated that the Hamiltonian preserves the coherence if it is an element of $\mathfrak{s}$, i.e. $H \in \mathfrak{s}$. Therefore, we expect that coherence breaking functions are elements of the algebra

$$\mathfrak{U} = \bigcup_{2 \leq p \leq k} \mathfrak{E}^{(p)}/\mathfrak{s}, \tag{895}$$

where k is a integer greater or equal to 2 and $\mathfrak{E}^{(p)}$ is the universal enveloping algebra of order p of the algebra $\mathfrak{g}$ corresponding to the Lie group G. In a visual way the universal enveloping algebra is the algebra build by all possible combinations and powers of the elements of the algebra $\mathfrak{g}$. The algebra $\mathfrak{U}$ is the universal enveloping algebra without the elements belonging to $\mathfrak{s}$. The universal enveloping algebra is infinite dimensional.

From soliton theory it is known that the coherent states for the infinite dimensional Lie algebra gl(∞) are given by the so-called τ-functions (set of all polynomial solutions to a hierarchy of equations encountered in soliton theory) [61]. The evolution of the τ-functions can be described by a succession of infinitesimal ***Bäcklund (contact) transformations***. Bäcklund transformations describe transformations between partial differential equations and their solutions. A well known example are the Cauchy-Riemann equations for the real and imaginary part of a holomorphic function. The real and imaginary part are both solutions of the Laplace equation and can be obtained from each other by harmonic conjugation, which in this case is the Bäcklund transformation. The fulfillment of the Laplace equation is a integrability criteria and tells us that they satisfy the Cauchy-Riemann equations. Also in a more general setting Bäcklund transformations are related with integrability conditions. We are interested in the question how we can substitute an infinite dimensional Lie algebra by a finite dimensional Lie algebra. This leads us to the framework of jet bundles.

Definition [175]: Jet Bundle I.0.1. *A jet bundle is a construction that makes a new smooth fibre bundle out of a given smooth fibre bundle. It makes it possible to write differential equations on sections of a fibre bundle in an (coordinate) invariant way. Given a m-dimensional manifold M, a fibre bundle (E, π, M), a multi-index $I = (I(1), \ldots, I(m))$ and let $\Gamma(\pi)$ denote the set of all local sections whose domain contains $p \in M$. We define*

$$|I| := \sum_{i=1}^{m} I(i), \quad \frac{\partial^{|I|}}{\partial x^I} := \prod_{i=1}^{m} \left(\frac{\partial}{\partial x^i} \right)^{I(i)}. \tag{896}$$

*For two local sections $\sigma, \eta \in \Gamma(\pi)$ we define the **r-jet** to be the equivalence class under the relation*

$$\frac{\partial^{|I|}\sigma^\alpha}{\partial x^I}\Big|_p = \frac{\partial^{|I|}\eta^\alpha}{\partial x^I}\Big|_p \tag{897}$$

with $0 < |I| < r$.

A system of non-linear partial differential equations of order s is equal to a submanifold $\mathscr{L}$ of a s-jet bundle $J^{(s)}$. The submanifold $\mathscr{L}$ is also equal to the zero set of a finitely generated ideal on functions on $J^{(s)}$ itself. If the integrability conditions of a map

$$\mathscr{B} : J^{(s)} \times \mathbb{R} \to J^{(1)} \tag{898}$$

comprise a system of differential equations on $J^{(s)} \times \mathbb{R}$, then $\mathscr{B}$ is a Bäcklund transformation. We can equip functions on $J^{(1)}$ with the infinite Lie algebra structure by the following construction. Consider a vector field $\mathscr{V}$ on $J^{(1)}$ defined by

$$\mathscr{V} \odot \vartheta = 0, \tag{899}$$

$$\mathscr{V} \odot \mathrm{d}\vartheta - \omega \quad \in \Omega^{(1)}, \tag{900}$$

where $\odot$ denotes the interior product, ϑ is a given contact 1-form over the smooth manifold E and ω is an arbitrary 1-form. The ***contact module*** $\Omega^{(s)}$ is defined by the pull-back from $J^{(s)}$ to $\mathbb{R}$ and if $t > s$, then $\Omega^{(s)}$ is a submodule of $\Omega^{(t)}$. If ω is an exact 1-form, that is $\omega = \mathrm{d}f$, where f is a function on $J^{(1)}$, then the Lie bracket is given by

$$[f, g] = \mathscr{V}_f g \tag{901}$$

for a function g on $J^{(1)}$ and we set $\mathscr{V} = \mathscr{V}_f$. In this case $\mathscr{B}$ is an automorphism of the defined Lie algebra structure.

Definition [176]: Contact Structure/Form I.0.2. *Given an n-dimensional smooth manifold M, and a point $p \in M$, a contact element of M with contact point p is an $(n-1)$-dimensional linear subspace of the tangent space to M at p.A contact structure on an odd dimensional manifold M, of dimension $2k+1$, is a smooth distribution of contact elements, denoted by ξ, which is generic at each point. The genericity condition is that ξ is non-integrable (there exist no invariant, regular foliations; i.e. ones whose leaves are embedded submanifolds of the smallest possible dimension that are invariant under the flow). A smooth distribution of contact elements ξ can locally be given by a differential 1-form, the contact form.*

Let K be a differential manifold and $T(K)$ be its tangent bundle and we define a map $a : K \to T(K)$. Let $F(K)$ be the algebra of smooth functions (C^∞) on K. The commutator in eq. (901) defines the gauge algebra $\mathscr{A}$ over K. The conditions on $\mathscr{V}_f$ imply that $\mathscr{V}_f$ is tangent to the fibres of a map $\pi : E \to K$ and we refer to the space of maps π by $\mathcal{E}$. The contact 1-form ϑ induces on $\mathcal{E}$ a contact 1-form ϑ_a by

$$\vartheta_a = \int_K \vartheta(a(p))\mathrm{d}\mu(p) \tag{902}$$

with $p \in K$ and $\mu(p)$ is a measure over K. The generators of the gauge current algebra $\mathscr{A}$ are in this case given by

$$\sigma_a = \int_K \gamma(p)a(p)\mathrm{d}\mu(p), \tag{903}$$

where $\gamma(p)$ is a bilinear map such that

$$[\sigma_a, \sigma_b] = c_{ab}\sigma_{a\circ b}, \quad c_{ab} \in \mathbb{C}. \tag{904}$$

Now we come to the ***prolongations*** [175]. The prolongations $\mathscr{B}^{(t)}$ are composed of maps of higher jet bundles and systems $\mathscr{L}^{(t)}$ of submanifolds induced form $\mathscr{B}$ and $\mathscr{L}$. In a coordinate description the prolongations $\mathscr{B}^{(t)}$ are just total derivatives. If there is an integer t such that the image of $\mathscr{B}^{(t)}$ and $\mathscr{L}^{(t)}$ is a new system of partial differential equations $\mathscr{L}'$ on $J^{(t+1)}$, then we have a Bäcklund map between the system of nonlinear partial differential equations $\mathscr{L}$ and the new system of partial differential equations $\mathscr{L}'$. In this case the Bäcklund maps are a generalization of ***contact transformations*** (transformations preserving a contact structure) and can be described by (local) diffeomorphisms of $J^{(1)}$ satisfying $\mathscr{B}^*\Omega^{(1)} = \Omega^{(1)}$, where $\mathscr{B}^*$ is a map of forms and functions induced from $\mathscr{B}$. The generalization are (local) diffeomorphisms of $J^{(s)}$ which preserve $\Omega^{(s)}$. It is possible to identify the components of cross sections from $T(K)$ to K with functions on $J^{(1)}$ by a suitable choice of the basis. Let $\mathfrak{l}$ be isomorphic to the gauge current algebra $\mathscr{A}$. It can be identified with a submodule of differential operators over the algebra $F(K)$ of C^∞ functions on K with compact support. The map π induces a new map $F(K) \to F(E)$ which makes it possible to identify $F(K)$ with a subring R_0 (ring = half group with respect to multiplication, that is there exists no inverse element) of $F(E)$. Let R_1 be the subspace of functions $f \in F(E)$, such that $\mathscr{V}_f$. We have the algebra

$$[R_0, R_0] = 0 \tag{905}$$
$$[R_1, R_0] \subset R_0, \quad [R_1, R_1] \subset R_1. \tag{906}$$

Then the Lie subalgebra $F^{(1)} = R_0 + R_1$ of $F(E)$ has a representation by first-differential operators on K [177].

Next we define a ***filtration*** $\{\mathfrak{l}^{(n)}\}$ of $\mathfrak{l}$ by $R_n = R_1 R_{n-1}$ for $n \geq 1$. The filtered algebra associated with R_n is $F^{(n)} = R_0 + \ldots + R_n$ and we have

$$\left[F^{(n)}, F^{(m)}\right] \subset F^{(n+m-1)}, \tag{907}$$

$$\left[\mathfrak{l}^{(n)}, \mathfrak{l}^{(m)}\right] \subset \mathfrak{l}^{(n+m-1)}. \tag{908}$$

We can define a subalgebra $\mathscr{L}_q$ of $\mathfrak{l}$ by

$$\mathfrak{L}_q = \bigcup_{n=q}^{\infty} \mathfrak{l}^{(n)}. \tag{909}$$

For the finite case the expression $\bigcup_{1\leq n\leq q}\mathfrak{l}^{(n)}$ is in general not a subalgebra of $\mathfrak{l}$ (only for $q=1$). In particular for $q\geq 1$, $\mathfrak{L}_q$ is an invariant subalgebra of $\mathfrak{L}_1$. This allows us to define the factor algebra

$$\mathfrak{I}_q = \mathfrak{L}_1/\mathfrak{L}_{q+1}, \quad \forall\, q \geq 1. \tag{910}$$

We denote the group obtained form the exponentiation of the algebra $\mathfrak{l}$ by $\mathscr{L}$ and its stabiliser subgroup by $\mathscr{I}$ with infinitesimal generators $\{\mathfrak{F}_l^{\Lambda_s}\}_{s=1}^q$, leaving a point $p\in K$ fixed. By Λ_s, $\overline{\Lambda}_{t-s}$ we denote the poly indices $\Lambda_s=\{l_1,\ldots l_s\}$, $\overline{\Lambda}_{t-s}=\{\bar{l}_{s+1},\ldots,\bar{l}_t\}$ for $t\geq s+1$. The algebra of the stabiliser subgroup is then given by

$$\left[\mathfrak{F}_l^{\Lambda_n},\mathfrak{F}_m^{\overline{\Lambda}_{t-n}}\right] = \delta_{l\bar{l}_s}\mathfrak{F}_m^{\overline{\overline{\Lambda}}_t\setminus\bar{l}_s} - \delta_{ll_r}\mathfrak{F}_m^{\overline{\Lambda}_t\setminus l_r}, \tag{911}$$

where $\overline{\overline{\Lambda}}_t=\Lambda_n\cup\overline{\Lambda}_{t-n}$, with $n\geq 1$, $t\geq n+1$, $n+1\leq s\leq t$ and $l\leq r\leq n$.

The $\{\mathfrak{F}_l^{\Lambda_s}\}_{s=1}^q$ form a representation of $\mathfrak{I}_q$. For given $n\geq 0$, let $\mathcal{I}^{(n)}$ be the subset of all $\mathfrak{F}_l^{\Lambda_n}$. Similiar to the grading of the $\mathfrak{l}$ we have

$$[\mathcal{I}^n,\mathcal{I}^m]\subset\mathcal{I}^{(n+m-1)}, \quad n>0. \tag{912}$$

However, $\mathcal{I}^{(0)}=\varnothing$ is the empty set and it is possible to set $\mathcal{I}^{(n)}=\varnothing$ for all n larger than a fixed integer k. This gives rise to the jet representation of order k of $\mathfrak{l}$

$$\mathscr{D}^{(k)}:\mathfrak{l}\to\bigcup_{n=1}^{k}\mathcal{I}^{(n)}, \quad \mathscr{D}^{(k)}(\sigma_a) = a\cdot\partial_p + \sum_{n=1}^{k}\sum_{l=1}^{\dim K}\sum_{\Lambda_n}\frac{1}{n!}c_a^{\Lambda_n}\mathfrak{F}_l^{\Lambda_n}, \tag{913}$$

with the coefficients $c_a^{\Lambda_n}=\frac{\partial^{L_n}a}{\partial p^{l_1}\ldots\partial p^{l_n}}\in\mathbb{C}$, where $L_n=\sum_{s=1}^n l_s$. In this representation $H+W$ preserves a set of coherent states $\tilde{G}_q$ obtained from an exponentiation of $\mathfrak{I}_q$. Only a set of coherent states of measure zero of the orbit of $\tilde{G}_q$ belongs to the orbit of G. ■

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