The Dynamics of Loop Quantum Gravity in the Cosmological and Semiclassical Sector from the Perspective of Reduced Quantisation and Extended Semiclassical Techniques

Die Dynamik der Schleifenquantengravitation im kosmologischen und semiklassischen Sektor aus der Perspektive reduzierter Quantisierung und erweiterter semiklassischer Techniken

Der Naturwissenschaftlichen Fakultät

der Friedrich-Alexander-Universität

Erlangen-Nürnberg

zur

Erlangung des Doktorgrades Dr. rer. nat.

vorgelegt von

David Winnekens

Als Dissertation genehmigt
von der Naturwissenschaftlichen Fakultät
der Friedrich–Alexander–Universität Erlangen–Nürnberg
Tag der mündlichen Prüfung: 07.06.2023

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In the beginning the Universe was created.
This has made a lot of people very angry and been widely regarded as a bad move.
There is a theory which states that if ever anyone discovers exactly what the Universe is for and why it is here, it will instantly disappear and be replaced by something even more bizarre and inexplicable.
There is another theory which states that this has already happened.

The Hitchhiker's Guide to the Galaxy
Douglas Adams

To Joachim, Katrin & Simone

Declaration

The work this thesis is based on was published in the following papers:

- *"A reduced phase space quantisation of a model in Algebraic Quantum Gravity with polarised* $\mathbb{T}^3$ *Gowdy symmetry"*, together with Kristina Giesel and Andreas Leitherer [1]
- *"Coherent States on the Circle: Semiclassical Matrix Elements in the Context of Kummer Functions and the Zak transformation"*, together with Kristina Giesel [2]
- *"Analysing (cosmological) singularity avoidance in loop quantum gravity using U(1)*^{3} *coherent states and Kummer's functions"*, together with Kristina Giesel [3]

Part II of this thesis covers the content of the first paper and Part III the remaining two. The text of these articles has been reused.
Sections of text within this thesis have been reused from an article published in *Classical and Quantum Gravity*. IOP Publishing Ltd is not responsible for any errors or omissions in the text included within this thesis. The Accepted Manuscript of the to be published article is available online at `https://doi.org/10.1088/1361-6382/acc0c7`.

Additionally, a fourth publication entitled *"Dynamics of Dirac observables in canonical cosmological perturbation theory"* was published by Kristina Giesel and Parampreet Singh together with the author [4]. As the content of that work is not closely related to the topics presented here, it is kept out of this thesis.

Co-Authorship Declaration

Contribution of David Winnekens to the publication „*Coherent States on the Circle: Semiclassical Matrix Elements in the Context of Kummer Functions and the Zak transformation*“, *arXiv e-prints* (https://arxiv.org/abs/2001.02755), to be submitted

As a co-author, I confirm that David Winnekens contributed significantly to the results of the publication above. This involves his 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. The presentation of the work in the thesis summarizes well his contributions to the publication.

Kristina Giesel

Contribution of David Winnekens to the publication „*Analysing (cosmological) singularity avoidance in loop quantum gravity using* $U(1)^3$ *coherent states and Kummer's functions*“, https://arxiv.org/abs/2109.07450, accepted by and to be published in *Classical and Quantum Gravity*

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Kristina Giesel

Contribution of David Winnekens to the publication „*A reduced phase space quantisation of a model in Algebraic Quantum Gravity with polarised* $\mathbb{T}^3$ *Gowdy symmetry*“, in preparation

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Andreas Leitherer

Acknowledgements

It is my great pleasure to say thank you to the people who joined me on my path towards finishing this thesis.

First of all, I am extremely grateful to Kristina Giesel, without whom this endeavour would not have been possible. It was a great pleasure to work with you, discuss all kind of different things — and find that last minus sign! Thank you for offering a helping hand or advice whenever needed and for all your fruitful inputs. I furthermore appreciate the freedom you gave me to also pursue new directions of our projects that I was interested in. I will always look back with joy on our work together!

I also want to thank Thomas Thiemann and Hanno Sahlmann for all the interesting discussions we had and your most helpful support on many occasions.
Thank you to Parampreet Singh for the fruitful collaboration on the dynamics of Dirac observables and likewise to Andreas and Refik for that on the Gwody models.
Furthermore, I want to thank Martina Gercke, Ursula Maerker, Gesine Murphy, Venetta Thompson, Jutta Zintchenko and all the staff of FAU's Department of Physics: both for always providing a helping hand and all the nice chats.

I am happy to extend my thanks to everyone of the Institute for Quantum Gravity with whom I shared some part of their university path: Alex, Almut, Andrea, Andreas, Antonia, Beatriz, Daniele, Klaus, Laura, Michael, Moritz, Refik, Robert, Simon, Susanne, Suzanne, Thomas and Thorsten. Be it table soccer matches, pub nights or barbecue on the terrace — there are a lot of memories to wallow in! I am furthermore happy for Juan having visited us, it was a great time and good fun with you.

I am also grateful for the joint coffee breaks with the "TheFeKöPhys" André, Barış, Christian, Jeremy, Pedro, Susi and Veronika, where we always had enjoyable and interesting conversations — and where I got some insight into your field, too.

Thank you to everyone of the Physicists' Football team, it was great fun!

I am very grateful to the *Studienstiftung des deutschen Volkes* (German Academic Scholarship Foundation), not only for the financial, but also for the ideational support throughout my university life and for all the good friends I made on numerous occasions.

Likewise, I am thankful for the FAU Erlangen–Nürnberg for both having provided a stipend to support this project as well as its *Leonardo-Kolleg* that supported my studies before.

I also want to say thank you to Michael Koehn for giving me enough freedom to finish this thesis during the years of our joint work.

Last but *of course* not least: I could not have undertaken this whole journey without the support of my family and further friends. Thank you especially to my parents Joachim and Katrin as well as my wife Simone.

The measure of a life is a measure of love and respect ⋄ *Neil Peart*

Abstract

The main object of investigation of this thesis was the cosmological and semiclassical realm of loop quantum gravity, which was addressed from two different directions. On the one hand, we analysed a cosmological toy model, and on the other hand a new procedure for conducting the computation of semiclassical expectation values was introduced. With the help of the latter, we revisited possible singularity avoidance in loop quantum gravity — which was so far only either analysed in so-called loop quantum cosmology, was limited to special configurations like cubic graphs, or was only possible by utilising estimations.

The cosmological toy model considered in this thesis, a so-called *Gowdy model*, features a $\mathbb{T}^3$ symmetry and is of special interest when the cosmological realm of (loop) quantum gravity shall be investigated as it still, despite its simplifications, yields a field theory after quantisation. Loop quantisations of such models relying on Dirac quantisation already exist in the literature. We extend those results by applying a reduced quantisation via coupling Gaussian dust to gravity as a dynamical reference frame. The quantisation is performed for two different frameworks: reduced loop quantum gravity and algebraic quantum gravity, where for both approaches a graph preserving prescription is applied. Analysing a Schrödinger-like equation and finding special solutions thereof then constitute first applications of this model. We find zero volume states and states that experience a vanishing action of the Euclidean part of the physical Hamiltonian. When it comes to the corresponding Lorentzian part, in turn, we analyse degeneracies caused by its action. Overall, these are first steps for gaining an overview over the different aspects of the action of the physical Hamiltonian of such $\mathbb{T}^3$ Gowdy models.

Addressing the question of singularity avoidance in full loop quantum gravity, we introduce a technique relying on *Kummer's confluent hypergeometric functions*. It turns out that they feature a lot of very handy properties like an asymptotic expansion for large arguments that allow for an exact calculation of certain semiclassical expectation values

by means of a power series in the semiclassicality parameter. These are taken of a specific class of operators that play a pivotal role in the dynamics of the theory and with respect to complexifier coherent states — the state-of-the-art coherent states used in loop quantum gravity. Seminal results of the literature that addressed singularity avoidance are generalised and extended with the help of this new method. Specifically, these improvements are that it is not always necessary to use estimates and that it is in fact possible to also conserve the correct powers of the momentum, e.g. The latter is also exemplified by applying the new procedure to standard quantum mechanics, where expectation values of fractional powers of the momentum operator can be computed analytically, resulting in a power series in $\hbar$.

On a more fundamental level, we use the Zak transformation to link coherent states on the circle to those of the harmonic oscillator. This further allows for a more efficient computation of (the zeroth order of) semiclassical matrix elements as we provide a link between semiclassical matrix elements in $L_2(\mathbb{R})$ and $L_2(S_1)$. What is more, also Kummer's confluent hypergeometric functions offer new insight on the fundamental level: As Kummer's differential equation can be linked to the heat equation, we can associate Kummer's confluent hypergeometric functions with solutions to the heat equation.

Zusammenfassung

Der Titel der Arbeit überträgt sich ins Deutsche als „Die Dynamik der Schleifenquantengravitation im kosmologischen und semiklassischen Sektor aus der Perspektive reduzierter Quantisierung und erweiterter semiklassischer Techniken“.

Der Fokus dieser Arbeit lag auf dem kosmologischen und semiklassischen Bereich der Schleifenquantengravitation, welcher von zwei Seiten beleuchtet wurde. Einerseits wurde ein kosmologisches Spielzeugmodell analysiert und andererseits eine neue Methode zur Berechnung semiklassischer Erwartungswerte eingeführt. Mit Hilfe des Letzteren wurde eine mögliche Aufhebung von Singularitäten in der Schleifenquantengravitation untersucht, was zuvor stets unter gewissen Einschränkungen geschah: Sei es, indem man sich im Rahmen der sogenannten Schleifenquanten*kosmologie* bewegte, indem man sich auf spezielle Konfigurationen wie kubische Graphen beschränken musste oder Abschätzungen verwendet hat.

Das kosmologische Spielzeugmodell, welches wir in dieser Arbeit betrachten – ein sogenanntes *Gowdy Modell* –, weist eine $\mathbb{T}^3$-Symmetrie auf und ist von besonderem Interesse, wenn man den kosmologischen Bereich der (Schleifen-)Quantengravitation untersuchen möchte. Dies liegt daran, dass es trotz der mit der $\mathbb{T}^3$-Symmetrie einhergehenden Vereinfachungen weiterhin eine Feldtheorie nach der Quantisierung hervorbringt. Schleifenquantisierungen solcher Modelle basierend auf Dirac Quantisierungen existieren bereits in der Literatur. Wir erweitern diese Resultate, indem wir eine reduzierte Quantisierung anwenden, für welche wir Gaußschen Staub an die Gravitation koppeln, den wir sodann als dynamischen Referenzrahmen verwenden. Diese Quantisierung erfolgte auf zweierlei Art: im Rahmen der reduzierten Schleifenquantengravitation sowie im Rahmen der algebraischen Quantengravitation – stets mittels Graph-erhaltender Quantisierungsvorschriften. Die ersten Anwendungen dieses Modells bestanden sodann aus der Analyse einer Schrödinger-ähnlichen Gleichung und der Konstruktion spezieller Lösungen hiervon. Insbesondere

fanden wir Zustände ohne Volumen, aber auch solche, die eine verschwindende Wirkung des euklidischen Teils des physikalischen Hamiltonians aufweisen. Bezüglich der Wirkung des lorentzschen Teils wiederum analysierten wir die auftretente Entartung. All dies sind erste Schritt, um einen Überblick über verschiedene Aspekte der Wirkung des physikalischen Hamiltonians eines solchen $\mathbb{T}^3$ Gwody Modells zu gewinnen.

Um die Vermeidung von Singularitäten in der (vollen) Schleifenquantengravitation zu untersuchen, führten wir eine neue Methode ein, die auf *Kummers konfluenten hypergeometrischen Funktionen* basiert. Diese besitzen einige äußerst praktische Eigenschaften, wie zum Beispiel ihre asymptotische Entwicklung für große Argumente, dank derer bestimmte semiklassische Erwartungswerte exakt als Potenzreihe im semiklassischen Parameter berechnet werden können. Diese Erwartungswerte wurden bezüglich sogenannter Komplexifizierer-kohärenter Zustände berechnet und von einer speziellen Klasse von Operatoren, welche für die Dynamik der Theorie von zentraler Bedeutung sind. Mit Hilfe dieser neuen Methode konnten wir sodann bereits existierende Ergebnisse erweitern und generalisieren, sodass wir beispielsweise nicht mehr notwendigerweise auf Abschätzungen zurückgreifen mussten und somit prinzipiell auch die anfänglichen Exponenten des Impulses während der Berechnungen beibehalten konnten. Letzteres zeigten wir exemplarisch auch am Beispiel der Quantenmechanik, wo wir Erwartungswerte von gebrochenen Potenzen des Impulsoperators berechneten und als Ergebnis eine Potenzreihe in $\hbar$ erhielten.
Auf fundamentalerer Ebene benutzten wir die Zak Transformation, um eine Beziehung zwischen kohärenten Zuständen auf dem Kreis und solchen des harmonischen Oszillators aufzuzeigen. Eine Verbindung zwischen semiklassischen Matrixlementen in $L_2(\mathbb{R})$ und $L_2(S_1)$ ermöglicht es insbesondere, semklassische Matrixelemente effizienter berechnen zu können. Darüber hinaus ermöglichen auch Kummers konfluente hypergeometrische Funktionen neue Einblicke auf fundamentaler Ebene: Wir zeigten einen Zusammenhang zwischen Kummers Differentialgleichung und der Wärmeleitungsgleichung, woduch Kummers konfluente hypergeometrische Funktionen als Lösungen der Wärmeleitungsgleichung verstanden werden können.

Introduction

Modern physics foots with the realms of quantum theory and general relativity on two columns that are for themselves very profound, but it is still not clear on which common theoretical foundation they stand. Their mathematical backgrounds are very different indeed, and yet we know they must — ultimately — be thought together, do we not only since the spectacular observations of the Event Horizon Telescope [5–10] know that objects exist that we assume to be situated in the realms of both these two branches. Finding a theory of *quantum gravity* is therefore unsurprisingly one of the main concerns of modern theoretical physics. Over the last decades, some ansätze arose, of which *string theory* certainly got the most attention so far.[1] The framework this thesis relies on, in turn, is called *loop quantum gravity* and follows a very different route. With string theory having its roots in particle physics, it replaces the point-like particles of the standard model with one-dimensional *strings* that — depending on the excitation of the string, much like a vibrating guitar string — carry the physical properties of one or the other elementary particle. For what is more, "supersymmetric" partners of the already known particles arise from the theory, where each bosonic elementary particle has a fermionic "superpartner" – and vice versa —, as well as a "graviton" that carries the gravitational force and thereby provides the link to gravity. In contrast, loop quantum gravity aims at directly quantising general relativity *as is*. While the details are outlined in Part I, we may give here a brief historical overview of how the field emerged, restricted to those findings that are most relevant for the work at hand.[2] The formulation of general relativity that constitutes the starting point of quantisation endeavours of gravity was first published in 1959 by Richard Arnowitt, Stanley Deser & Charles W. Misner [15], now known as the so-called "ADM formalism" after their initials. It offers a Hamiltonian description of gravity

[1] Please refer to [11, Introduction and Sec. 4.1 & 5.1] or [12, App. B] for a broader overview.

[2] There are of course many more publications and people that were important for the development of the field. For more comprehensive overviews, see references of [1] as well as [13], with its chapter on the history of loop quantum gravity being available online, too [14].

by introducing a 3-1 split of spacetime into three spatial and one temporal dimension. While this split is essential for a quantum theory relying on *canonical* quantisation, it also respects the fundamental principles of general relativity by keeping the split arbitrary without preferring the one or the other frame of reference. In contrast, the *covariant* description of loop quantum gravity, so-called *spin foam models*, does not need such a split [16–18].

Based on work from the early 1980s by Amitabha Sen [19, 20], who introduced using connections as field variables, Abhay Ashtekar [21, 22] in the mid- to late 1980s realised that this allows to describe general relativity by means of a new set of canonical variables in Yang–Mills style, which also casts the Hamiltonian constraint — one of the fundamental quantities — into polynomial form. These new variables are now referred to as the Ashtekar–Barbero variables, honouring also the work of Fernando Barbero who proceeded the formalism towards real-valued connections [23, 24]. It was then Ted Jacobson, Carlo Rovelli and Lee Smolin [25, 26] who realised that these new variables can be used to apply a canonical quantisation prescription relying on Wilson loops to quantum gravity, which was introduced already in 1980 for Yang–Mills theories by Rodolfo Gambini & Antoni Trias [27]. It then followed a fruitful phase of many important works on this loop representation and we suggest the interested read to consult the book of Rodolfo Gambini & Jorge Pullin [28] for a broad overview. From this point on — having a well understood loop representation for quantum gravity at hand —, many progress was possible, culminating i.a. in the construction of the kinematical Hilbert space and essential proofs of its properties by Abhay Ashtekar, Christopher Isham, Jerzy Lewandowski, Donald Marolf, José Mourão and Thomas Thiemann in [29–34] as well as a well-defined Hamiltonian constraint operator constructed by Thomas Thiemann in 1996 [35].

A theory of quantum gravity, as mentioned above, is expected to shed a new light on extreme objects like black holes, but new insights are also expected concerning the Big Bang. To proceed into this direction, Martin Bojowald and Hans Kastrup introduced *loop quantum cosmology* in 1999 / 2000 [36–40]. Within this framework, it was possible to indeed resolve the Big Bang singularity [41–45]. However, this result should only be regarded as a first step towards singularity avoidance in full (loop) quantum gravity. Loop quantum cosmology is based on a quantisation of symmetry reduced general relativity with finitely many degrees of freedom, so it is not a priori clear whether its results also transfer to the whole theory. Work by i.a. Norbert Bodendorfer, Johannes Brunnemann, Jonathan Engle, Christian Fleischhack, Maximilian Hanusch, Tim Koslowski and Thomas

Thiemann discuss how loop quantum cosmology may be embedded into loop quantum gravity [46–52].
Such a resolution of the Big Bang singularity was also observed by Daniele Oriti, Lorenzo Sindoni & Edward Wilson-Ewing [53] in a framework called *group field theory* — to learn more about it, we refer to beautiful publications by Laurent Freidel [54] and Daniele Oriti [55]. Concerning the singularity resolution in group field theory, [56, Footnote 14 & context] notes that it is wholly different to that within loop quantum cosmology: In group field theory, the continuous shrinking is prohibited by a "sort of 'quantum pressure'", which "can be traced back to a never-vanishing number density [...], rather than to the discreteness of volume spectrum or absence of zero eigenvalues from it" [56] as it is the case in loop quantum cosmology. Very much contrary to loop quantum cosmology, the singularity resolution also exists in group field theories with continuous volume spectrum [57].
In (full) loop quantum gravity, in turn, addressing these questions is a lot harder. It is this tension between working in the full theory — where calculations quickly become very involved — and working in a toy model — where one may have chosen too drastic simplifications — where the work of the thesis at hand aims to take a grip and offer new insights as well as new techniques for how to tackle some of the obstacles that come up.

Goal of the thesis

The goal of the thesis at hand is twofold. On the one hand, Part II covers so-called Gowdy models. These are cosmological models, but their properties are not linked to those of the observable universe. They are instead of interest as they still yield a field theory upon quantisation while also allowing for conducting computations too complex in the full theory. This makes them a good toy model or playground for new methods to develop or test. One such framework that we will apply to Gowdy models is so-called *algebraic quantum gravity*, published by Kristina Giesel and Thomas Thiemann in 2006 [58–61]. Within this framework, we then aim at implementing first applications like finding zero volume states or solutions to a Schrödinger-like equation.

Part III, on the other hand, then focuses on addressing singularity avoidance via the semiclassical sector. This approach is based on a class of coherent states introduced in loop quantum gravity by Thomas Thiemann in 2002[3] [62]. Together with Hanno Sahlmann [63, 64], first results on calculating specific semiclassical expectation values that play a pivotal role in the quantum dynamics were published. Johannes Brunnemann and Thomas Thiemann [65, 66], in turn, analysed singularity avoidance using these coherent states and utilising chains of estimates in order to be able to solve these computations at the analytical level. We want to look at these seminal works from a different angle by applying a new semiclassical technique relying on *Kummer's confluent hypergeometric functions*.

This thesis therefore aims at adding new insights to both these branches: assessing singularity avoidance via semiclassical computations as well as further developing the treatment of Gowdy models within loop quantum gravity in order to be able to construct and better understand novel (cosmological or semiclassical) techniques. All the aforementioned steps, frameworks and techniques will be introduced in more detail within the respective parts and chapters.

Results

When it comes to the treatment of Gowdy models in loop quantum gravity, the existing literature mainly consists of hybrid quantisation techniques — a mixture of a quantisation à la loop quantum gravity for the homogeneous modes and a Fock quantisation for the inhomogeneous ones. The latter part makes it then hard to compare these models to ones that do not use a Fock quantisation. The literature also offers a few non-hybrid quantisation ansätze for Gowdy models, using a Dirac quantisation instead. However, the resulting quantum dynamics obtained via Dirac quantisation is so complex that the respective physical Hilbert space has not yet been constructed for these models. In contrast, the reduced quantisation performed in this thesis offers a direct access to the physical Hilbert space for such Gowdy models. The regularisation within the quantisation procedure introduced in the work presented here also allows for a graph-preserving action in both the loop quantum gravity as well as the algebraic quantum gravity framework. The dynamics can then be implemented via a Schrödinger-like equation within the algebraic quantum gravity approach. Due to the graph-preserving quantisation, the construction of solutions of the dynamics is technically simpler than in a model with graph-modifying

[3]The publication year of the online preprint https://arxiv.org/abs/gr-qc/0206037

operators. As a first step, we construct very specific solutions of the Schrödering-like equation. Their purpose is mainly to show how one can work with the involved operators, understand their actions and to outline techniques that help constructing more general solutions in future work.

The results on semiclassical computations are twofold itself. On the one hand, we en route extended results from the literature on coherent states on the circle, linking semiclassical matrix elements of $L_2(S_1)$ and $L_2(\mathbb{R})$ via the Zak transformation. This allows for a more efficient computation of these expressions. The main result especially for the loop quantum gravity framework, meanwhile, is the introduction of a new semiclassical technique relying on *Kummer's confluent hypergeometric functions*. This procedure allowed us to calculate semiclassical expectation values with respect to certain coherent states for an important class of dynamical operators that include fractional powers of momentum-like operators. While existing approaches into this direction had to rely on estimates or consider cubic graphs only, the new technique offers more freedom. Limitations enter when, for example, singularity avoidance should be analysed, enforcing the usage of estimates. However, even then the new approach offers improvements as information on the fractional power included in these operators is not lost. In standard quantum mechanics, Kummer's confluent hypergeometric functions enable the computation of semiclassical expectation values of fractional powers of the momentum operator in terms of a power series in $\hbar$.

Note that there are longer elaborations on the motivation, goals and results of the topics at the beginning and ending of their respective parts. We refer the reader interested in those summaries to Chapter 3 on *page 49* for Gowdy models and Chapter 9 *p. 121* for the semiclassical considerations. The conclusions of the two parts are found in Chapter 8 *p. 115* and, respectively, in Chapter 17 *p. 231* for the semiclassical part. We also provide a final conclusion in Chapter 18 *p. 239*.

Structure of the thesis

The work at hand is divided into three parts. Part I first of all offers an introduction into loop quantum gravity. It also covers techniques that will be later used in the investigations of Part II and Part III, like algebraic quantum gravity in Section 2.6 *p. 38* and (complexifier) coherent states in Section 2.7 *p. 39*.

As already mentioned, the following two parts on Gowdy models and semiclassical considerations each include their own introductory chapters on motivation and goals as well as concluding summaries.

Part II continues with the discussion of $\mathbb{T}^3$ Gowdy models. After an introductory chapter on the motivation of the work, Chapter 4 *p. 53* introduces the classical setup, where the symmetry reduction to the $\mathbb{T}^3$ Gowdy model is outlined in Section 4.2 *p. 55*. Chapter 5 *p. 59* and Chapter 6 *p. 79* are then similar in structure and concept: They present the quantisation of the $\mathbb{T}^3$ Gowdy model in the reduced loop quantum gravity setup and the algebraic quantum gravity framework, respectively. The respective first sections set the mathematical background, followed by the quantisation of the Euclidean and Lorentzian parts in the subsections of Section 5.2 *p. 64* and Section 6.2 *p. 83*, respectively. The first applications performed in the algebraic quantum gravity setting of the $\mathbb{T}^3$ Gowdy model are then presented in Chapter 7 *p. 89*: A Schrödinger-like equation is set up in Section 7.1 *p. 89*, where we first investigate the action of the main components of the physical Hamiltonian on the basis states in Subsection 7.1.1 *p. 92*, then introduce an ansatz for Gowdy states in Subsection 7.1.2 *p. 93* and analyse the action of the physical Hamiltonian thereon in Subsection 7.1.3 *p. 97*. Afterwards, in Section 7.2 *p. 102*, we discuss specific solutions of the Schrödinger-like equation, starting with zero-volume eigenstates in Subsection 7.2.1 *p. 103*. We also outline a generalisable procedure for finding specific solutions therein. Continuing, in Subsection 7.2.2 *p. 104*, we construct Gowdy states that experience a vanishing action of the Euclidean part of the Hamiltonian. The Lorentzian part of the Hamiltonian is then examined in Subsection 7.2.3 *p. 110*, where we analyse degeneracies of its action on the Gowdy states.

Part III then covers the semiclassical investigations. The overall setup, the operators of interest and some special methods like the Poisson resummation formula are introduced in Chapter 10 *p. 129*. Chapter 11 *p. 135* covers Kummer's confluent hypergeometric functions and some of their (for our purpose) most important properties. Using standard quantum mechanics, we furthermore show in Section 11.3 *p. 139* how these functions can be used to calculate semiclassical expectation values of fractional powers of the momentum operator, but also of more complex operators that mimic the one later used in the loop quantum gravity scenario. The chapter concludes in Section 11.4 *p. 144* with a comparison of the new method with one from the literature, introduced in the algebraic quantum gravity framework. We continue by considering Kummer's confluent hypergeometric functions in the context of coherent states on the circle in Chapter 12 *p. 147*. These allow to compute semiclassical expectation values, as presented in Subsection 12.2.1 *p. 154*. Subsection 12.2.2 *p. 157* then revisits the Zak transformation for linking semiclassical matrix elements of $L_2(S_1)$ and $L_2(\mathbb{R})$. Another aspect where Kummer's confluent hypergeometric functions can be used to gain new insights is discussed in this chapter's last section, Section 12.4 *p. 165*, where we present a connection between Kummer's differential equation and the heat equation. Chapter 13 *p. 169* then carries over this new procedure to the loop quantum gravity scenario. We start the new computations within loop quantum gravity in Chapter 14 *p. 173* with focusing on cubic graphs. Therein, Section 14.2 *p. 175* presents the analytical computation of the basic building block of the expectation values of interest and Section 14.3 *p. 184* offers a first remark on (cosmological) singularity avoidance. In the last section of this chapter, Section 14.4 *p. 186*, we show that Kummer's confluent hypergeometric functions allow for retrieving the correct semiclassical continuum limit for cubic graphs. Graphs with higher valent vertices are then covered in Chapter 15 *p. 189* and Chapter 16 *p. 203*. First, Chapter 15 *p. 189* generalises an analytic procedure from the literature, which was introduced for cubic graphs, and compares it to the technique using Kummer's confluent hypergeometric functions. Then, Chapter 16 *p. 203* addresses more general configurations of the operators within the semiclassical expectation values, making it necessary to introduce estimates. Accordingly, we first of all recap estimative procedures from the literature in Section 16.1 *p. 204* and adapt them to the approach via Kummer's confluent hypergeometric functions. Finally, in Section 16.2 *p. 213*, we elaborate on finding new estimates that potentially refine the previously obtained results and which conditions they have to fulfil — guided by new insights gained from the procedure via Kummer's confluent hypergeometric functions.

Part I

Loop Quantum Gravity

Chapter 1

Introductory remarks

This first part shall provide an introduction into *loop quantum gravity* — the basis of all the considerations of this thesis. Loop quantum gravity aims at providing a quantum theory of gravity. It does so by quantising general relativity without adding any further structure and without understanding quantum gravity as a perturbative phenomenon. Loop quantum gravity is therefore a background-independent theory. While it is not necessary to introduce new structure to the theory, describing loop quantum gravity in higher dimensions and with supersymmetry in order to find a connection to string theory was indeed approached in a series of papers by Norbert Bodendorfer, Thomas Thiemann & Andreas Thurn [67–75]. This indicates that loop quantum gravity can be extended to loop quantum *super*gravity.

What will be introduced in the following chapter is the *canonical* framework of loop quantum gravity. There also exists the *covariant* framework — a treatment of loop quantum gravity motivated by the Feynman path integral formalism — whose main subject are so-called *spin foams*. However, as the considerations of this thesis will not touch this area and an additional introduction into this approach would nevertheless need much space, we refrain from doing so and refer the interested reader to a review by Alejandro Perez and introductions by John Baez [16–18]. For literature also covering the further development of this theory, please consider the books by Carlo Rovelli and Carlo Rovelli & Francesca Vidotto [12, 76] or the recent review by Sebastian Steinhaus [77].

Chapter 2

Framework

2.1 Hamiltonian general relativity and the ADM formalism

The ADM formalism — named after Richard Arnowitt, Stanley Deser & Charles W. Misner [15] — is the natural starting point of this thesis as it is the underlying Hamiltonian description of general relativity (GR) behind all subsequent considerations and for building a quantum theory of GR in particular. Its quintessence is a 3+1 split of the four-dimensional spacetime in order to be able to obtain a Hamiltonian formalism — that at the very heart of it needs an entity, regarded as "time", along which the system will evolve. Note that this naming is only due to the fact that this variable is used to describe the evolution of the system, while all further physical interpretations one associates with "time" are not necessarily satisfied as well. While [15] initially considered ${}^{(3)}g_{ab} := g_{ab}$ as the spatial metric,[1] it has become standard [11] to choose the more general induced metric q_{ab} on a three-dimensional space-like submanifold Σ: We understand the four-dimensional spacetime manifold $\mathcal{M}$ as a direct product $\mathcal{M} \cong \mathbb{R} \times \Sigma$ that is globally hyperbolic. The latter is important as it ensures a unique solution for the initial value problem. Using X^μ as coordinates on $\mathcal{M}$ and x^a on Σ, we can define this embedding via

$$\forall t \in \mathbb{R}, X_t \colon \Sigma \to \mathcal{M} : X_t(\vec{x}) := X(\vec{x}, t), \tag{2.1}$$

[1] Note that we use Greek indices $\mu, \nu, \ldots = 0, 1, 2, 3$ for the whole spacetime and Latin indices $a, b, \ldots = 1, 2, 3$ for spatial coordinates. The ${}^{(3)}$ denotes a quantity defined on a 3-dimensional manifold.

where the X^μ are collected in X and the x^a in $\vec{x}$. This leads to a foliation of spacetime into spatial slices $\Sigma_t := X_t(\Sigma)$ of constant time, see Figure 2.1.

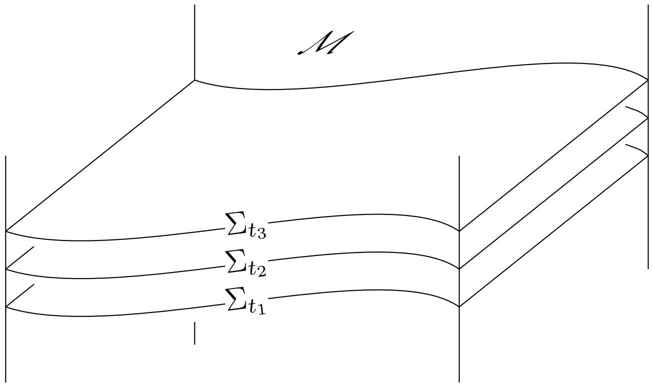

Figure 2.1: Foliation of $\mathcal{M}$ into space-like slices Σ_t

Note that changing from one foliation to another can be achieved by applying a diffeomorphism — just concatenate the new foliation with the current one's inverse, which is a diffeomorphism. Accordingly, acting with a diffeomorphism can also be understood as just changing the foliation.

On these hypersurfaces Σ_t, we can define the precursors of the desired spatial metric q_{ab} and the extrinsic curvature K_{ab} of Σ: the first and the second fundamental form

$$q_{\mu\nu} := g_{\mu\nu} + n_\mu n_\nu \text{ and} \tag{2.2}$$

$$K_{\mu\nu} := q^\rho_\mu q^\sigma_\nu \nabla_\rho n_\sigma \tag{2.3}$$

respectively, where we used the standard covariant derivative of $g_{\mu\nu}$, ∇_μ, and $q_{\mu\nu} = g_{\mu\rho} q^\rho_\nu$, i.e. raising and lowering of indices is still performed via $g_{\mu\nu}$ — except for solely spatial objects, where we can of course also use $q_{\mu\nu}$. n^μ is a normalised vector perpendicular to Σ_t, arising via the definition of the deformation vector field

$$T^\mu(X) := \frac{\partial X^\mu(\vec{x}, t)}{\partial t} =: N(X) n^\mu(X) + N^\mu(X). \tag{2.4}$$

N^μ then is tangential to Σ_t and we have a decomposition of T^μ into a part normal to Σ_t and one tangential to it. To word these quantities meaningfully, N is called the *lapse function* and N^μ the *shift vector field*.

We can now already start to calculate all the important geometrical quantities in their spatial projection. For example, the Gauß–Codazzi equation applied to this scenario tells us the Riemann curvature on Σ_t, as described via the four-dimensional one of $\mathcal{M}$:

$$^{(3)}R_{\mu\nu\rho\sigma} = q^{\alpha}_{\mu} q^{\beta}_{\nu} q^{\gamma}_{\rho} q^{\delta}_{\sigma} \, ^{(4)}R_{\alpha\beta\gamma\delta} - 2K_{\rho[\mu} K_{\nu]\sigma}. \tag{2.5}$$

This yields directly

$$^{(3)}R \coloneqq q^{\mu\rho} q^{\nu\sigma} \, ^{(3)}R_{\mu\nu\rho\sigma} = q^{\mu\rho} q^{\nu\sigma} \, ^{(4)}R_{\mu\nu\rho\sigma} - K^2 + K_{\mu\nu} K^{\mu\nu} \tag{2.6}$$

for the spatial Ricci scalar $^{(3)}R$, where $K \coloneqq q^{\mu\nu} K_{\mu\nu}$. With this, we see that we can almost describe the classical Einstein–Hilbert action

$$S_{\mathrm{EH}} \coloneqq \frac{1}{\kappa} \int\limits_{\mathcal{M}} \mathrm{d}^4 X \sqrt{|\det g|} \, ^{(4)}R \tag{2.7}$$

in terms of the 3+1 decomposition, i.e. separate spacetime and formulate $^{(4)}R$ in terms of 3+1 quantities only. In the equation above, we defined $\kappa \coloneqq 16\pi G$ with Newton's constant G. What is now left is to replace the spacetime Riemann curvature tensor by the corresponding spacetime Ricci scalar by means of

$$^{(4)}R = g^{\mu\rho} g^{\nu\sigma} \, ^{(4)}R_{\mu\nu\rho\sigma} = q^{\mu\rho} q^{\nu\sigma} \, ^{(4)}R_{\mu\nu\rho\sigma} - 2n^{\nu} [\nabla_\mu, \nabla_\nu] n^{\mu}, \tag{2.8}$$

via the split according to (2.2), and finally pull everything back to Σ. Yet again, we first of all perform further modifications before treating the pullback and replace the last term, via expanding the commutator, by

$$2n^{\nu} [\nabla_\mu, \nabla_\nu] n^{\mu} = -2K_{\mu\nu} K^{\mu\nu} + 2K^2 + 2\nabla_\mu (n^\nu \nabla_\nu n^\mu - n^\mu \nabla_\nu n^\nu). \tag{2.9}$$

Plugging (2.9) into (2.8) and the result into (2.6), we obtain this scenario's version of the Codazzi relation:

$$^{(4)}R = {}^{(3)}R - K^2 + K_{\mu\nu} K^{\mu\nu} - 2\nabla_\mu (n^\nu \nabla_\nu n^\mu - n^\mu \nabla_\nu n^\nu). \tag{2.10}$$

If we now think about inserting this into the Einstein–Hilbert action, we recognise the last term to be a boundary term that we can neglect from now on (for a more detailed elaboration on this, see Subsection 1.5.1 in [11] and the bountiful references therein). We then proceed with the last step: As we ultimately want to have a description on $\mathbb{R} \times \Sigma$ at hand, i.e. in coordinates $(\vec{x}, t)$, we can now define the already mentioned spatial metric q_{ab} together with the pulled back extrinsic curvature K_{ab}. They are described by means of the initial spacetime metric $g_{\mu\nu}$ according to

$$q_{ab}(\vec{x}, t) \coloneqq (X^\mu_a X^\nu_b q_{\mu\nu})(X(\vec{x}, t)) = (X^\mu_a X^\nu_b g_{\mu\nu})(X(\vec{x}, t)) \text{ and} \tag{2.11}$$

$$K_{ab}(\vec{x}, t) \coloneqq (X^\mu_a X^\nu_b K_{\mu\nu})(X(\vec{x}, t)) = (X^\mu_a X^\nu_b \nabla_\mu n_\nu)(X(\vec{x}, t)), \tag{2.12}$$

where we defined

$$X^\mu_a \coloneqq X^\mu_{,a} \coloneqq \frac{\partial X^\mu}{\partial x^a}, \tag{2.13}$$

i.e. a set of three tangential vectors that together with n^μ build a frame.

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※ As a side note: Looking at (2.11), we can now understand the initial usage of ${}^{(3)}g_{ab} = g_{ab}$ in [15]: If we want $q_{ab} \equiv {}^{(3)}g_{ab} = g_{ab}$, we need $X^\mu_a = \delta^\mu_a$. We get this by simply taking over the orientation of the spatial part of the spacetime basis for the new spatial hypersurfaces, see Figure 2.2.[2] Generally, one obtains an angle between associated pairs of axes, depicted by the grey areas. However, one can make them overlap via rotations to get the intrinsic convention of the original ADM work.

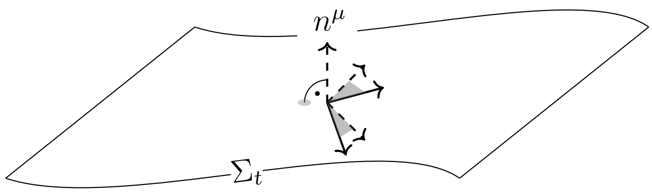

Figure 2.2: Orientation of the bases of the spatial part of spacetime (dashed lines) and the spatial hypersurface (solid lines)

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[2]There, only two spatial dimensions are considered. The last and all in all fourth dimension is left to the advanced reader's imagination.

Let's go back to describing the necessary quantities pulled back to Σ. For the lapse function N and the shift vector $\vec{N}$, we have

$$N(\vec{x},t) := N(X(\vec{x},t)) \text{ and} \tag{2.14}$$
$$N^a(\vec{x},t) := q^{ab}(\vec{x},t)(X^\mu_b g_{\mu\nu} N^\nu)(X(\vec{x},t)), \tag{2.15}$$

respectively, and for the contracted extrinsic curvature and the spatial Ricci scalar

$$K(\vec{x},t) = \big(q^{ab}K_{ab}\big)(\vec{x},t) \text{ and} \tag{2.16}$$
$$\begin{aligned} R(\vec{x},t) &:= {}^{(3)}R(\vec{x},t) \\ &= q^{ab}(\vec{x},t)q^{cd}(\vec{x},t)\big(X^\mu_a X^\nu_b X^\rho_c X^\sigma_d {}^{(3)}R_{\mu\rho\nu\sigma}\big)(X(\vec{x},t)). \end{aligned} \tag{2.17}$$

Note that we may now raise and lower these purely spatial indices via the spatial q_{ab}.

Combining all the previous results, we may now rewrite the Einstein–Hilbert action in 3+1 form, called the ADM action:

$$S_{\mathrm{EH}} = \frac{1}{\kappa}\int\limits_{\mathcal{M}} \mathrm{d}^4X \sqrt{|\det g|}\, {}^{(4)}R \tag{2.18}$$
$$= \frac{1}{\kappa}\int\limits_{\mathbb{R}} \mathrm{d}t \int\limits_{\Sigma} \mathrm{d}^3x \sqrt{|\det q|}\; |N| \big(R + K_{ab}K^{ab} - K^2\big) =: S_{\mathrm{ADM}}. \tag{2.19}$$

The consequent next step is to proceed with the Hamiltonian description of GR in terms of the just introduced ADM formalism. In order to perform the initial Legendre transformation, we make use of

$$K_{ab} = \frac{1}{2N}\big(\dot{q}_{ab} - (\mathcal{L}_{\vec{N}}q)_{ab}\big), \tag{2.20}$$

linking K_{ab} with both the temporal and the Lie derivative $\mathcal{L}_{\vec{N}}$ of q, what allows us to determine the set

$$P^{ab}(\vec{x},t) := \frac{\delta S_{\mathrm{ADM}}}{\delta \dot{q}_{ab}}(\vec{x},t) = \frac{|N|}{N\kappa}\sqrt{|\det q|}\big(K^{ab} - q^{ab}K\big) \tag{2.21}$$
$$\Pi(\vec{x},t) := \frac{\delta S_{\mathrm{ADM}}}{\delta \dot{N}}(\vec{x},t) = 0 \tag{2.22}$$
$$\Pi_a(\vec{x},t) := \frac{\delta S_{\mathrm{ADM}}}{\delta \dot{N}^a}(\vec{x},t) = 0 \tag{2.23}$$

of canonically conjugate momenta of the variables q_{ab}, N and N^a. The last two equations tell us that we face a constrained Hamiltonian system with the primary constraints

$$C(\vec{x},t) \coloneqq \Pi(\vec{x},t) = 0 \text{ and} \tag{2.24}$$

$$C_a(\vec{x},t) \coloneqq \Pi_a(\vec{x},t) = 0. \tag{2.25}$$

With these primary constraints entering our setup, we are forced to proceed via Dirac's algorithm for constrained systems [78], telling us to include these constraints with associated Lagrange multipliers $\lambda(\vec{x},t)$ and $\lambda^a(\vec{x},t)$ in the primary Hamiltonian density. This leads us to

$$S = \int_{\mathbb{R}} \mathrm{d}t \int_{\Sigma} \mathrm{d}^3x \Big(\dot{q}_{ab} P^{ab} + \dot{N}\Pi + \dot{N}^a \Pi_a - \lambda C - \lambda^a C - NH - N^a D_a \Big), \tag{2.26}$$

along finding the so-called *Hamiltonian constraint* H and the spatial *diffeomorphism constraints* D_a:

$$H \coloneqq \frac{\kappa}{\sqrt{|\det q|}} \left(q_{ac} q_{bd} - \frac{1}{2} q_{ab} q_{cd} \right) P^{ab} P^{cd} - \frac{\sqrt{|\det q|}}{\kappa} R \quad \text{and} \tag{2.27}$$

$$D_a \coloneqq -2 q_{ac} \, \mathcal{D}_b \, P^{bc}. \tag{2.28}$$

They arise by enforcing the stability condition on the primary constraints, i.e. that their temporal derivatives vanish, too. In the above, $\mathcal{D}_a$ is the covariant derivative metric compatible with q via

$$\mathcal{D}_a \, q_{bc} = 0 \tag{2.29}$$

and defined by

$$\mathcal{D}_a \, v^b \coloneqq \partial_a v^b + \Gamma^b{}_{ac} v^c, \tag{2.30}$$

where $\Gamma^b{}_{ac}$ are the (spatial) Christoffel symbols.

We can now also state the Hamiltonian of the system,

$$\mathbf{H} \coloneqq \frac{1}{\kappa} \int_{\Sigma} \mathrm{d}^3x (\lambda C + \lambda^a C_a + |N| H + N^a D_a), \tag{2.31}$$

which turns out to be composed of constraints only. This gives rise to the so-called *problem of time*, which we will discuss in more detail in Section 2.5.

For now, with this Hamiltonian at hand, the next step of Dirac's algorithm is to check the stability of the primary constraints: As we demand them to be fulfilled at any instant of time, their vanishing alone is not sufficient. We also need their temporal derivative to vanish, and hence their evolution to be trivial:

$$\dot{C} := \{C, \mathbf{H}\} \approx 0 \text{ and } \dot{C}_a := \{C_a, \mathbf{H}\} \approx 0. \tag{2.32}$$

Before continuing with the stability analysis of the constraints, we may introduce the notion of *first class* and *second class constraints*. First of all, the sign $\approx$ symbolises the notion of *being fulfilled weakly*: The corresponding equation holds with an $=$ only on the *constraint hypersurface* — the hypersurface on which all constraints are fulfilled. A first class constraint then is one that has a weakly vanishing Poisson bracket with all other constraints of the theory, i.e. it is vanishing on the constraint hypersurface. We will see that all Poisson brackets between constraints are again proportional to constraints: $\{H(|N'|), \mathbf{H}\} \approx 0$. Hence, in our case, we have at hand a set of first class constraints. A second class constraint then is one that has a non-vanishing (not even weakly) Poisson bracket with at least one of the remaining constraints.

Now, at this point of the stability analysis, one typically goes over to use the so-called smeared constraints

$$C(N') := \int_\Sigma \mathrm{d}^3x\, N'(\vec{x},t) C(\vec{x},t) \text{ and} \tag{2.33}$$

$$\vec{C}\left(\vec{N}'\right) := \int_\Sigma \mathrm{d}^3x\, \vec{N}'(\vec{x},t) \vec{C}(\vec{x},t) = \int_\Sigma \mathrm{d}^3x\, N'^a(\vec{x},t) C_a(\vec{x},t), \tag{2.34}$$

which can also be generalised with arbitrary smearing functions $f(\vec{x},t)$ and $f^a(\vec{x},t)$ instead of lapse and shift. Their advantage is that using them avoids singular Poisson brackets and we get as stability conditions the set

$$\{C(N'), \mathbf{H}\} = H(|N'|) \tag{2.35}$$

$$\left\{\vec{C}\left(\vec{N}'\right), \mathbf{H}\right\} = \vec{D}\left(\vec{N}'\right). \tag{2.36}$$

Consequently, we understand the Hamiltonian and (spatial) diffeomorphism constraints as secondary constraints — enforcing the stability of the primary constraints —, hence demanding

$$H \approx 0 \text{ and } D_a \approx 0 \tag{2.37}$$

to ensure the stability of the primary constraints. Yet again, we have to check their stability by calculating the set [11, (1.2.14)]

$$\{H(|N'|), \mathbf{H}\} = H(\mathcal{L}_{\vec{N}}|N'|) - \vec{D}\Big(\vec{M}(|N'|, |N|, q)\Big) \tag{2.38}$$

$$\Big\{\vec{D}\Big(\vec{N'}\Big), \mathbf{H}\Big\} = -H(\mathcal{L}_{\vec{N'}}|N|) - \vec{D}\Big(\mathcal{L}_{\vec{N'}}\vec{N}\Big), \tag{2.39}$$

where we used the abbreviation $M^a(|N'|, |N|, q) := q^{ab}(|N'|\partial_b|N| - |N|\partial_b|N'|)$. Noticing that the right hand sides are composed of constraints only, we do not need to impose tertiary constraints and their stability is ensured from this point onwards.

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※ As a side note: The above set of Poisson brackets is an immediate consequence of the more general Dirac algebra [78], also referred to as the hypersurface deformation algebra [11].[3] There, one uses the more general ansatz of smearing the constraints with arbitrary test functions f and f^a instead of lapse and shift. The three possible combinations of the two smeared constraints put into Poisson brackets then reveal

$$\{H(f), H(f')\} = -\kappa\vec{D}\Big(\vec{M}(f, f', q)\Big), \tag{2.40}$$

$$\Big\{\vec{D}\Big(\vec{f}\Big), \vec{D}\Big(\vec{f'}\Big)\Big\} = -\kappa\vec{D}\Big(\mathcal{L}_{\vec{f}}\vec{f'}\Big) \text{ and} \tag{2.41}$$

$$\Big\{H(f), \vec{D}\Big(\vec{f}\Big)\Big\} = \kappa H\Big(\mathcal{L}_{\vec{f}}f\Big). \tag{2.42}$$

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These two sets of Poisson brackets show an important aspect, that is the algebras tell us the constraint hypersurface is invariant under the action of the constraints.

[3]Note, however, that it is in fact not a genuine Lie algebra as it does not contain structure constants but structure functions.

Summarising the procedure so far, we performed a 3+1 split of spacetime into a three-dimensional manifold Σ and the one-dimensional $\mathbb{R}$ — the first we regard as the spatial realm and the latter serves as the "time" line. Since we keep this split completely arbitrary by not further specifying N or N^μ, we do not break general covariance. For globally hyperbolic manifolds, we can always choose a foliation Σ_t of the four-dimensional spacetime (cf. fig. 2.1) and changing from one foliation to another is equivalent to applying a diffeomorphism. The aim was then to rewrite the Einstein–Hilbert action in quantities that reflect this 3+1 split. We pulled back the relevant geometrical quantities to Σ, like the Ricci scalar, and found the ADM action of GR, (2.19). With this formal introduction of (a notion of) time, we proceeded with performing the Legendre transformation in order to find the Hamiltonian description. It turned out that GR is in fact a fully constrained Hamiltonian system and we had to include the primary constraints C and C_a in the Hamiltonian (2.31).

2.2 Ashtekar variables and the birth of loop quantum gravity

In a paper published in 1986, Ashtekar introduced "new variables for classical and quantum gravity" [21]. With their help, he achieved to tackle several issues of the framework up to this point, but also managed to link GR to Yang–Mills theory. The footing of the new variables is the so-called tetrad formalism [79]. By choosing four vector fields as a basis — hence "tetrads" —, one can reformulate $g_{\mu\nu}$ and any other tensors in terms of them. We explain this adopted to the ADM framework. There, we face the three-dimensional sub-manifold Σ, asking for three "triads" e_i. We introduce the new notation via the identities

$$e^i_a e^b_i = \delta^b_a \quad \text{and} \quad e^i_a e^a_j = \delta^i_j. \tag{2.43}$$

The indices a and b are the usual spatial indices ranging from 1 to 3. The range of the indices i and j is also from 1 to 3, but they are abstract SO(3)-indices, referred to as "internal" ones.[4] They are called that way as they do not posses any "real" or physical interpretation in the sense that the other sets of indices (of spacetime $\mathcal{M}$ or the spatial

[4]From now on, Latin characters from i onwards denote internal SU(2)-indices and Latin characters from the beginning of the alphabet mark spatial indices on Σ.

sub-manifold Σ) do and are merely relevant for actions within their symmetry group. Describing the spatial metric in terms of the co-dreibein,[5]

$$q_{ab} \coloneqq \delta_{ij} e^i_a e^j_b, \tag{2.44}$$

we can now understand the underlying SU(2)-symmetry. While q_{ab} is fixed, we have the freedom of changing/rotating the triads in SU(2)-space. This opposition is resolved by introducing a new constraint, but we will come to that later.

Due to the introduction of this additional structure, the new configuration space is obviously larger, which gives rise to the so-called *extended* phase space. Thereon, the conjugate variable for the triad is

$$K^i_a \coloneqq K_{ab} e^b_i. \tag{2.45}$$

Note that the correct index notation would be $e^{b\,i}$, but since we raise and lower internal indices via the SU(2) Cartan metric δ^i_j, we might as well use the more pleasing e^b_i and omit the delta for brevity. We will henceforth ignore stringent positions of internal indices when necessary regarding this aspect.

In order to obtain simpler expressions in what follows, one proceeds with

$$E^a_i \coloneqq \sqrt{\det q}\, e^a_i \tag{2.46}$$

as the densitised representative of the triad. We then indeed have

$$\begin{aligned} \big\{E^a_i(x), K^j_b(y)\big\} &= \frac{\kappa}{2}\delta^a_b \delta^j_i \delta(x,y) \quad \text{and} \\ \big\{E^a_i(x), E^b_j(y)\big\} &= 0 = \big\{K^i_a(x), K^j_b(y)\big\}, \end{aligned} \tag{2.47}$$

with the Hamiltonian and the diffeomorphism constraints reading

$$H = \frac{1}{\sqrt{\det q}}\big(K^i_a K^j_b - K^j_a K^i_B\big) E^a_j E^b_i - \sqrt{\det q}\, R \quad \text{and} \tag{2.48}$$

$$D_a = 2\,\mathcal{D}_a\big(K^i_c E^c_i\big) - 2\,\mathcal{D}_b\big(K^i_a E^b_i\big), \tag{2.49}$$

respectively. Note that the covariant derivative above is symbolised by an upright $\mathcal{D}$, in

[5] "Dreibein" is just another frequently used name for the triads, derived from the German word for *tripod*.

contrast to the italic D of the diffeomorphism constraint. The appearance of a new kind of indices now asks for a generalised form of this covariant derivative that not only acts on the spatial but also sees these abstract indices — as in (2.49) above, if $\mathcal{D}_a$ acts on the single factors of the two products. We use the same symbol $\mathcal{D}_a$ and just extend its method of operation on objects with both kinds of indices:

$$\mathcal{D}_a\, T_i^b \coloneqq \big(\mathcal{D}_a\, T^b\big)_i + \left(\mathcal{D}_a\, T_i\right)^b \coloneqq \big(\partial_a T^b + \Gamma^b{}_{ac} T^c\big)_i + \big(\partial_a T_i + \Gamma_{ai}{}^j T_j\big)^b. \tag{2.50}$$

Note that the spatial covariant derivative, i.e. the first term in parentheses, equals (2.30). In addition to the Christoffel symbol $\Gamma^b{}_{ac}$, there is now a new object $\Gamma_{ai}{}^j$. We notice it contains both spatial and internal indices and due to the latter it is called *spin connection*. The new adapted "metric" compatibility then reads

$$\mathcal{D}_a\, e_b^i = 0 \tag{2.51}$$

and

$$\mathcal{D}_a\, E_i^a = \partial_a E_i^a + \epsilon_{ij}{}^k \Gamma_a^j E_k^a = 0 \tag{2.52}$$

for the densitised triad. From (2.51), we can directly derive the elements of the spin connection via (2.50),

$$\Gamma_{ai}{}^j = -\big(\partial_a e_i^b + \Gamma^b{}_{ac} e_i^c\big) e_b^j, \tag{2.53}$$

and then use these to introduce

$$\Gamma_a^i \coloneqq \epsilon^{ijk} \Gamma_{ajk}. \tag{2.54}$$

In terms of the densitised triad, its components read [11]

$$\Gamma_a^i = \frac{1}{2}\epsilon^i{}_j{}^k E_k^b \big(E_{a,b}^j - E_{b,a}^j + E_j^c E_a^l E_{c,b}^l\big) + \frac{1}{4}\epsilon^i{}_j{}^k E_k^b \frac{2E_a^j (\det E)_{,b} - E_b^j (\det E)_{,a}}{\det E}. \tag{2.55}$$

Additional to the two familiar constraints above, there is now a new one — answering the unphysical degrees of freedom of rotating the triads regarding their internal indices. We can infer from (2.45) that due to the symmetry of K_{ab}, there needs to be an equivalent condition for K_a^i — the rotational constraint

$$G_{ij} \coloneqq K_{a[i} E_{j]}^a = 0. \tag{2.56}$$

We will already entitle this constraint as *Gauß constraint*, though the origin of this naming will become clear only later — where we will also reformulate it in a more appropriate one-index fashion in (2.71).

All the above results in describing the status quo via the action

$$S = \frac{1}{\kappa} \int_{\mathbb{R}} \mathrm{d}t \int_{\Sigma} \mathrm{d}^3x \Big(2E^a_i \dot{K}^i_a - \big(NH + N^a D_a - \Lambda^{ij} G_{ij} \big) \Big), \tag{2.57}$$

where we had to include the new Gauß constraint with an appropriate antisymmetric smearing matrix Λ such that

$$\{G(\Lambda), G(\Lambda')\} = \frac{\kappa}{2} G([\Lambda, \Lambda']) \tag{2.58}$$

holds for the smeared Gauß constraint $G(\Lambda) = \int_\Sigma \mathrm{d}^3x \Lambda^{ij} G_{ij}$.

※ Before we proceed, we would like to check whether we still describe the same physics. Going back to (2.44), we see that we can express q_{ab} in terms of the triad (and hence the densitised triad) and obtain the conjugate variables

$$q_{ab} = |\det E| E^i_a E^i_b \quad \text{and} \tag{2.59}$$

$$P^{ab} = \frac{2}{|\det E|} E^a_i E^c_i E^d_j K^j_{[c} \delta^b_{d]}. \tag{2.60}$$

While the Gauß constraint commutes with q_{ab} due to rotational invariance in the abstract SO(2) indices, its fulfilment (2.56) reduces the second equation above to (2.21) and we recover the familiar pair of variables from the ADM formalism. We can then also check their Poisson brackets:

$$\{q_{ab}(x), q_{cd}(y)\} = 0, \tag{2.61}$$

$$\big\{P^{ab}(x), P^{cd}(y)\big\} = -\kappa \mathcal{G}^{abcd}(x) \delta(x,y) \approx 0 \quad \text{and} \tag{2.62}$$

$$\big\{P^{ab}(x), q_{cd}(y)\big\}) = \kappa \delta^a_{(c} \delta^b_{d)} \delta(x,y). \tag{2.63}$$

Therein, we collected all appearances of the Gauß constraint in the function $\mathcal{G}$. Hence, the corresponding Poisson bracket between two P is only weakly vanishing, i.e. on the constraint hypersurface defined by the Gauß constraint being fulfilled.

This tells us that working with the extended phase space and performing a symplectic reduction with respect to the Gauß constraint is equivalent to the description by means of the ADM variables.

Up to now, we constructed the new canonical conjugate pair (E^a_i, K^i_a), being subject to the additional Gauß constraint via their internal indices i. With (2.54) and a rescaling à la

$$
{}^{(\beta_{\mathrm{BI}})}K^i_a := \beta_{\mathrm{BI}} K^i_a \tag{2.64}
$$

$$
{}^{(\beta_{\mathrm{BI}})}E^a_i := \frac{1}{\beta_{\mathrm{BI}}} E^a_i, \tag{2.65}
$$

we arrive at the Ashtekar variables $\left({}^{(\beta_{\mathrm{BI}})}A^i_a, {}^{(\beta_{\mathrm{BI}})}E^a_i\right)$, with the Sen–Ashtekar–Immirzi–Barbero connection [20, 21, 80, 81]

$$
{}^{(\beta_{\mathrm{BI}})}A^i_a := \Gamma^i_a + {}^{(\beta_{\mathrm{BI}})}K^i_a. \tag{2.66}
$$

The rescaling coefficient β_{BI} is referred to as the Barbero–Immirzi parameter [24, 80] and is kept arbitrary; $\beta_{\mathrm{BI}} \in \mathbb{C} \setminus 0$.[6] With the new connection Γ^i_a containing triads and co-triads to the same degree, it is not affected by the rescaling via β_{BI} and therefore does not need to carry the preceding superscript (β_{BI}). These Ashtekar variables then form a pair of canonically conjugate variables:

$$
\left\{{}^{(\beta_{\mathrm{BI}})}A^i_a(x), {}^{(\beta_{\mathrm{BI}})}A^j_b(y)\right\} = 0 = \left\{{}^{(\beta_{\mathrm{BI}})}E^a_i(x), {}^{(\beta_{\mathrm{BI}})}E^b_j(y)\right\} \tag{2.67}
$$

$$
\left\{{}^{(\beta_{\mathrm{BI}})}E^a_i(x), {}^{(\beta_{\mathrm{BI}})}A^j_b(y)\right\} = \frac{\kappa}{2}\delta^a_b \delta^j_i \delta^{(3)}(x-y). \tag{2.68}
$$

While the previous pair of canonically conjugate variables (K^i_a, E^a_i) obeyed the desired Poisson bracket relations already (cf. (2.47)) the Hamiltonian and diffeomorphism constraints (2.48) & (2.49) take a better accessible form in the new Ashtekar variables: We formulated general relativity as an SU(2) gauge Yang–Mills theory, as we will discuss below. The Gauß constraint, on the other side, can be cast into a form that motivates that naming. We will now address the formulation of the constraints in the new variables.

[6] Note that there are preferred choices for the value β_{BI} takes. [82], e.g., showed that $\beta_{\mathrm{BI}} = \frac{\ln 2}{\pi\sqrt{3}}$ reproduces the Bekenstein–Hawking entropy for black holes.

2.2.1 The constraints

We first turn towards the Gauß constraint. Its current form (2.56) can be rewritten as

$$G_{ij} \coloneqq K_{a[i}E^a_{j]} = 0 \quad \Leftrightarrow \quad G_i = \epsilon_{ij}{}^k K^j_a E^a_k = 0. \tag{2.69}$$

We can then transfer the metric compatibility of (2.52) from E^i_b to ${}^{(\beta_{\mathrm{BI}})}E^i_b$ and obtain

$$\mathcal{D}_a\, {}^{(\beta_{\mathrm{BI}})}E^a_i = \partial_a {}^{(\beta_{\mathrm{BI}})}E^a_i + \epsilon_{ij}{}^k \Gamma^j_a\, {}^{(\beta_{\mathrm{BI}})}E^a_k = 0. \tag{2.70}$$

Adding this expression to the Gauß constraint, we notice that the term on the right hand side of (2.69) together with the second term of (2.70) combine for an expression $\sim {}^{(\beta_{\mathrm{BI}})}A^j_a$ and we can reformulate the Gauß constraint as

$$G_i = \partial_a {}^{(\beta_{\mathrm{BI}})}E^a_i + \epsilon_{ijk} {}^{(\beta_{\mathrm{BI}})}A^j_a {}^{(\beta_{\mathrm{BI}})}E^a_k =: {}^{(\beta_{\mathrm{BI}})}\mathcal{D}_a\, {}^{(\beta_{\mathrm{BI}})}E^a_i = 0. \tag{2.71}$$

This form now justifies the titling *Gauß* constraint. Proceeding with the remaining Hamiltonian and diffeomorphism constraint, we first of all define the curvature, or field strength tensor of Yang–Mills type, ${}^{(\beta_{\mathrm{BI}})}F^i_{ab}$ as follows:

$${}^{(\beta_{\mathrm{BI}})}F^i_{ab} \coloneqq \partial_a {}^{(\beta_{\mathrm{BI}})}A^i_b - \partial_b {}^{(\beta_{\mathrm{BI}})}A^i_a + \epsilon^i{}_{jk} {}^{(\beta_{\mathrm{BI}})}A^j_a\, {}^{(\beta_{\mathrm{BI}})}A^k_b. \tag{2.72}$$

By means of the curvature, we then find more compact forms of the Hamiltonian and diffeomorphism constraints [11]:

$$H = \left[\beta^2_{\mathrm{BI}}\, {}^{(\beta_{\mathrm{BI}})}F^i_{ab} - \left(\beta^2_{\mathrm{BI}} + 1\right)\epsilon^i{}_{jk} {}^{(\beta_{\mathrm{BI}})}K^j_a {}^{(\beta_{\mathrm{BI}})}K^k_b\right] \frac{\epsilon_i{}^{lm}\, {}^{(\beta_{\mathrm{BI}})}E^a_l {}^{(\beta_{\mathrm{BI}})}E^b_m}{\sqrt{|\beta^3_{\mathrm{BI}} \det {}^{(\beta_{\mathrm{BI}})}E|}} = 0 \tag{2.73}$$

$$D_a = {}^{(\beta_{\mathrm{BI}})}F^i_{ab} {}^{(\beta_{\mathrm{BI}})}E^b_i = 0. \tag{2.74}$$

Note that, as an intermediate step, one arrives at descriptions of these constraints that also include terms proportional to the Gauß constraint. However, with the Gauß constraint forming a subalgebra within the constraint algebra, we can drop these contributions [11].

With all the above, we can rewrite the Einstein–Hilbert action à la

$$S = \frac{1}{\kappa} \int\limits_{\mathbb{R}} \mathrm{d}t \int\limits_{\Sigma} \mathrm{d}^3x \Big(2\, {}^{(\beta_{\mathrm{BI}})}E^a_i\, {}^{(\beta_{\mathrm{BI}})}\dot{A}^i_a - \big(NH + N^a D_a - \Lambda^i G_i\big)\Big). \tag{2.75}$$

2.2.2 The holonomy–flux algebra

We notice that the appearance of delta distributions in the Poisson bracket structure (2.67) & (2.68) of the canonically conjugate pair of variables $\left({}^{(\beta_{\mathrm{BI}})}A^i_a, {}^{(\beta_{\mathrm{BI}})}E^a_i\right)$ makes them singular. To avoid this, it is a natural choice to proceed with smeared analogues. As we want the basic variables to reflect the SU(2) gauge transformations caused by the Gauß constraint, their algebra to close and additionally do not want them to rely on the metric as a background field — what, in turn, is often used for other Yang–Mills theories but is clearly inapplicable when the metric is one of the central dynamical quantities as it is for a theory of quantum gravity —, it turns out that the only solution are holonomies or so-called Wilson loops [11].
With the notation becoming more and more evolved, we may from now on omit the superscripts ${}^{(\beta_{\mathrm{BI}})}$ of ${}^{(\beta_{\mathrm{BI}})}A$ and ${}^{(\beta_{\mathrm{BI}})}E$.

Having a curve $c\colon [0,1] \to \Sigma$ lying in the spatial part Σ of the manifold $\mathcal{M}$, a holonomy $h_c(A)$ of a connection A along that curve reads

$$h_c(A) \coloneqq \mathcal{P}\exp\left(\int_c A\right) = \mathbb{1}_{\mathrm{SU}(2)} + \sum_{n=1}^{\infty} \int_0^1 \mathrm{d}t_1 \int_{t_1}^1 \mathrm{d}t_2 \ldots \int_{t_{n-1}}^1 \mathrm{d}t_n A(c(t_1)) \cdots A(c(t_n)) \tag{2.76}$$

and is uniquely defined by the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}\eta} h_{c_\eta}(A) = h_{c_\eta}(A) A^i_a(c(\eta)) \frac{\tau_i}{2} \dot{c}^a(\eta) \tag{2.77}$$

with the initial condition

$$h_{c_0}(A) = \mathbb{1}_{\mathrm{SU}(2)}. \tag{2.78}$$

Therein, we used $\tau_i = -\mathrm{i}\sigma_i$ as a basis of $\mathfrak{su}(2)$ with the well-known Pauli matrices σ_i. With $c_\eta(t) \coloneqq c(\eta t)$, for $\eta \in [0,1]$, it follows $h_{c_1}(A) \eqqcolon h_c(A)$. The conjugate variable then is the flux

$$E_n(S) \coloneqq \int_S n^i \epsilon_{abc} E^a_i \, \mathrm{d}x^b \wedge \mathrm{d}x^c, \tag{2.79}$$

where we integrate over an oriented two-dimensional surface $S \in \mathcal{M}$ and n is a (Lie algebra valued) smearing field.

The Poisson bracket of the two variables

$$\{E_n(S), h_c(A)\} = \frac{\beta\kappa}{2} n^i \tau_i h_c(A) \tag{2.80}$$

then is indeed not singular anymore and closes. Note that the above only holds if the normal of S shows in the same direction as the tangent of c does, whereas we get an additional minus sign if they show in opposite directions. If c does not intersect S at all, the Poisson bracket vanishes.

To complete the algebra of the constraints, which we already touched on for the Hamilton and diffeomorphism constraints (the hypersurface deformation algebra), i.e. to include the Gauß constraint as well, we first define the smeared constraints:

$$H(N) := \int_\Sigma H(x)N(x)\,\mathrm{d}^3x, \tag{2.81}$$

$$D\left(\vec{N}\right) := \int_\Sigma D_a(x)N^a(x)\,\mathrm{d}^3x \quad \text{and} \tag{2.82}$$

$$G(\Lambda) := \int_\Sigma G_i(x)\Lambda^i(x)\,\mathrm{d}^3x, \tag{2.83}$$

where $M^a(N, N', q) := q^{ab}(N\partial_b N' - N'\partial_b N)$ as before. We then get the full algebra of the constraints:

$$\{H(N), H(N')\} = \frac{\kappa^2\beta_{\mathrm{BI}}^2}{4}\vec{D}\left(\vec{M}(N, N', q)\right), \tag{2.84}$$

$$\left\{D\left(\vec{N}\right), H(N)\right\} = -H(\mathcal{L}_{\vec{N}}N), \tag{2.85}$$

$$\left\{D\left(\vec{N}\right), D\left(\vec{N}'\right)\right\} = -D\left(\mathcal{L}_{\vec{N}'}\vec{N}\right), \tag{2.86}$$

$$\{G(\Lambda), G(\Lambda')\} = \frac{\kappa}{2}G([\Lambda, \Lambda']), \tag{2.87}$$

$$\{G(\Lambda), H(N)\} = 0 \quad \text{and} \tag{2.88}$$

$$\left\{G(\Lambda), D\left(\vec{N}\right)\right\} = -G(\mathcal{L}_{\vec{N}}\Lambda). \tag{2.89}$$

This is the formulation of GR that we want to quantise. However, there is not *the one way* to quantise a system, especially when it comes to constraints involved in the theory.

2.3 The two paths of quantisation

Let us now approach the quantisation of the constraints G_i (2.71), D_a (2.74) and H (2.73), obeying the Dirac algebra (2.84) – (2.89). When quantising a system subject to constraints, there is a decision one has to make right at the beginning: Should one first solve the constraints in the classical theory and subsequently quantise the *reduced* theory, or, the other way around, first quantise the whole theory and then solve the constraints on the operator level. The first approach is known as *reduced phase space quantisation*, while the latter is referred to as *Dirac quantisation*. Figure 2.3 illustrates the different steps one has to carry out for these two very distinct paths. Details will become more clear during the treatment of the next sections, but this figure already motivates that these two routes are indeed quite different. As for the Dirac quantisation, one of the hardest tasks surely is finding the joint kernel of the quantised constraint operators — and thereby proceed from the *kinematical* to the *physical Hilbert space*. When it comes to the reduced phase space quantisation, it is the search for appropriate reference fields and a representation of the then obtained observable algebra that is responsible for the most effort. So there really is no universally preferred choice between the two of them — the conservation of difficulty — and for some scenarios it may even be best practice to mix them: Solve some of the constraints classically and then proceed with a Dirac quantisation of the remaining ones (see, e.g., the models outlined in [83]).

Since quantising first feels like the more canonical way to proceed, we start with this approach and then, in Section 2.5, delve into the reduced phase space quantisation, which the treatment of Chapter II relies on.

2.4 Dirac quantisation

We will start with introducing the notion of the basis states and the representation of the kinematical Hilbert space. The quantisation procedure will then be outlined for the Hamiltonian constraint and, before, for the volume operator, where we also include a small discussion on its importance as it will be on the heart of many considerations in the course of this work.

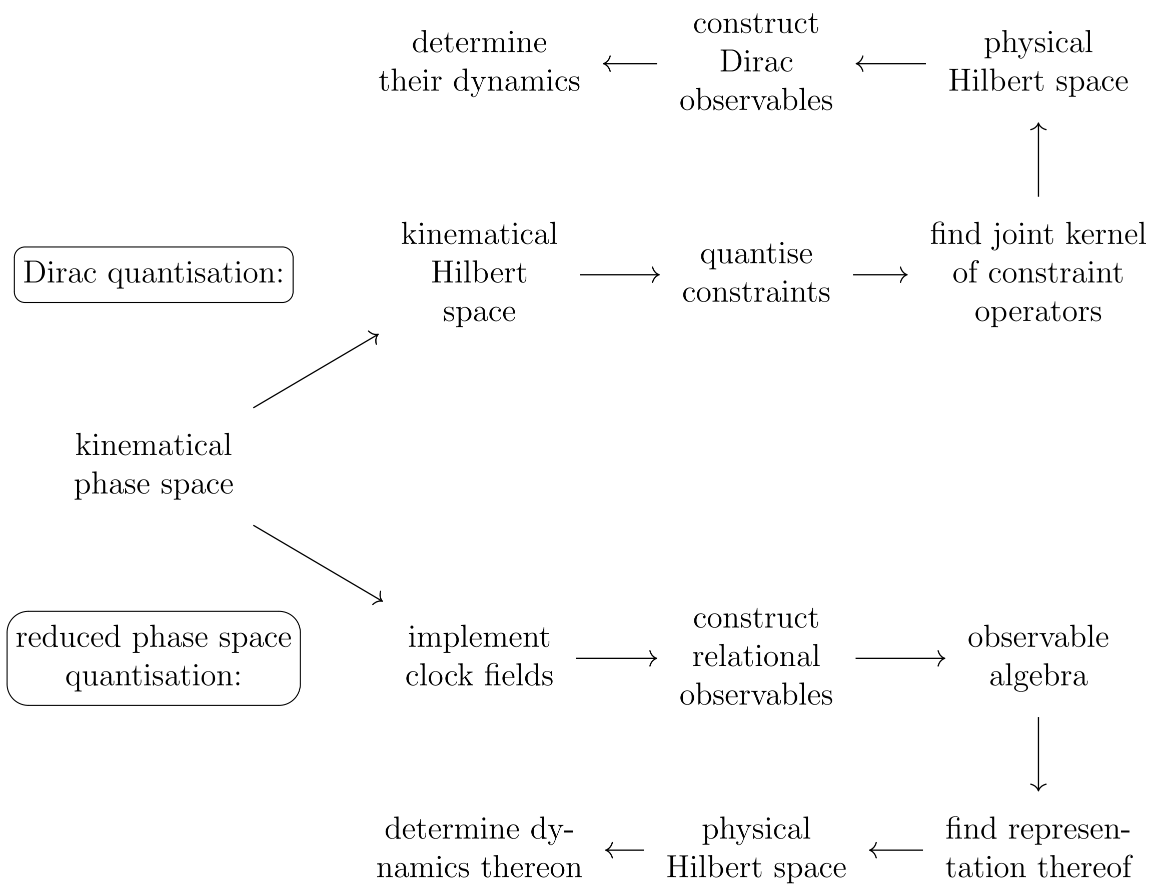


Figure 2.3: Basic steps of the Dirac and reduced phase space quantisation procedure

2.4.1 Spin network functions and the Ashtekar–Lewandowski representation

The functions that serve as basis states for the theory are the so-called *spin network functions* $T_\gamma(A)$ [84–86]. They are cylindrical functions of the holonomies $h_c(A)$ defined on an underlying graph γ that is embedded in the spatial manifold. The curves c the connection A is integrated along then are the graph's edges e_I and we denote by $E(\gamma)$ the set of all edges of a graph γ. Being a cylindrical function defined on a graph constituted of $M = |E(\gamma)|$ many edges means that the structure of the associated spin network function is edge-wise and reads

$$T_\gamma(A) = T_\gamma(h_{e_1}(A), h_{e_2}(A), \dots, h_{e_M}(A)). \tag{2.90}$$

On the level of the holonomies, we can therefore define the map

$$T_\gamma \colon \mathrm{SU}(2)^M \to \mathbb{C}, \tag{2.91}$$

for which we use the same notation. The kinematical Hilbert space of the theory then is

$$\mathcal{H}_{\mathrm{kin}} = L^2\big(\overline{\mathcal{A}}, \, \mathrm{d}\mu_{\mathrm{AL}}\big), \tag{2.92}$$

where $\overline{\mathcal{A}}$ is the space of generalised connections and $\mathrm{d}\mu_{\mathrm{AL}}$ the Ashtekar–Lewandowski measure. This Hilbert space is equipped with the inner product

$$\langle T_\gamma | T'_\gamma \rangle = \int\limits_{\mathrm{SU}(2)^M} \overline{T_\gamma(h_{e_1}, \dots, h_{e_M})}\, T'_\gamma(h_{e_1}, \dots, h_{e_M}) \, \mathrm{d}\mu_{\mathrm{H}}(h_{e_1}) \cdots \mathrm{d}\mu_{\mathrm{H}}(h_{e_M}), \tag{2.93}$$

where $\mathrm{d}\mu_{\mathrm{H}}$ denotes the SU(2) Haar measure. In the above, we assumed both spin network functions to be defined on the same graph. This, of course, is not necessarily true in general and if one in fact faces two different graphs γ_1 and γ_2, one proceeds with the union graph $\gamma = \gamma_1 \cup \gamma_2$. Last but not least, a point of a graph is called *vertex* v_I when at least two edges — which are not trivial extensions of each other — meet there. We collect all vertices of a graph in the set $V(\gamma)$.

The spin network functions then carry one irreducible representation of SU(2) on each edge, labelled by $j_e \; \forall e \in E(\gamma)$. We may collect those in the vector $\vec{j}$. On the vertices, in turn, so-called *intertwiners* I_v sit. These tensors knit the representations of all ingoing edges together with the ones of all outgoing edges and are collected in the vector $\vec{I}$. Hence, besides γ, spin network functions also carry the labels $\vec{j}$ and $\vec{I}$. In the literature, those are then often combined into a set, say $s = \left\{\gamma, \vec{j}, \vec{I}\right\}$, used as a labelling of the states. The notation T_γ at hand only considers the label γ for illustrating the graph structure of the spin network functions while omitting $\vec{j}$ and $\vec{I}$, but the difference between T_γ and T'_γ in (2.93) is precisely that of different $\vec{j}, \vec{I}$ and $\vec{j}', \vec{I}'$ — we just use a more concise notation. For a more detailed introduction of spin network states see e.g. [17, 84] or Chapter 32 of [11].

Acting on these basis states are the fundamental operators of the holonomy and the flux:

$$(\pi_{\mathrm{AL}}(h_e)\, T_\gamma)(A) = \hat{h}_e(A) T_\gamma(A) = h_e(A) \cdot T_\gamma(A) \quad \text{and} \tag{2.94}$$

$$(\pi_{\mathrm{AL}}(E_n(S))\, T_\gamma)(A) = \hat{E}_n(S) T_\gamma(A) = -\mathrm{i}\hbar \hat{\Delta} T_\gamma(A) \tag{2.95}$$

$$= -\frac{{\ell_{\mathrm{P}}}^2 \beta_{\mathrm{BI}}}{4} \sum_{v \in V(\gamma)} n^i(v) \sum_{e \ni v} \epsilon(e,S) \hat{J}_i^{(v,e)} T_\gamma(A). \tag{2.96}$$

This representation π_{AL} is called the Ashtekar–Lewandowski representation and from the equations above it looks quite similar to the action of the familiar Schrödinger representation. However, the $\hat{J}_i^{(v,e)}$ above is not just the right-invariant vector field on SU(2), i.e. a differential operator, but instead — due to the cyclic composition of the spin network functions —

$$\hat{J}_i^{(v,e)} = \mathbb{1}_{\mathrm{SU}(2)} \otimes \mathbb{1}_{\mathrm{SU}(2)} \otimes \cdots \otimes \left\{ \begin{matrix} \hat{X}_i^{(e)} \\ {}^{(L)}\hat{X}_i^{(e)} \end{matrix} \right\} \otimes \mathbb{1}_{\mathrm{SU}(2)} \otimes \cdots , \tag{2.97}$$

where now $\hat{X}_i^{(e)}$ and ${}^{(L)}\hat{X}_i^{(e)}$ indeed are the right- and left-invariant vector fields

$$\left(\hat{X}_i^{(e)} f\right)(h_e) := \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)_{t=0} f\left(\mathrm{e}^{t\tau_j} h_e\right) \quad \text{and} \tag{2.98}$$

$$\left({}^{(L)}\hat{X}_i^{(e)} f\right)(h_e) := \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)_{t=0} f\left(h_e \mathrm{e}^{t\tau_j}\right). \tag{2.99}$$

The right-invariant vector field acts on the spin network functions as

$$\left(\hat{X}_i^{(e)} T_\gamma\right)\left(h_{\{e\}}\right) = \mathrm{tr}\left((\tau_i h_e)^{\mathrm{T}} \frac{\partial}{\partial h_e} \right) T_\gamma\left(h_{\{e\}}\right) \tag{2.100}$$

and is replaced by the left-invariant vector field ${}^{(L)}\hat{X}_i^{(e)}$ in (2.97) if the edge e is ingoing at v. In the above, tr denotes the SU(2)-trace. Lastly, the function $\epsilon(e,S)$ in (2.96) accounts for the orientation of the edge with respect to the (oriented) surface S:

$$\epsilon(e,S) = \begin{cases} -1 & \text{if } e \text{ is below } S, \\ 0 & \text{if } e \cap S = \{\} \text{ or } \dot{e}(e \cap S) \in S, \\ 1 & \text{if } e \text{ is above } S. \end{cases} \tag{2.101}$$

Note that any arbitrary edge can be understood as a concatenation of edges of these types.

With this, we face the familiar situation of one multiplicatively and one differentially acting operator associated with the basic quantities. When it comes to the action of some physically intuitive operators built from these basic ones, however, the obtained consequences turn out to be not as familiar anymore — as the next section shows.

2.4.2 Geometrical Operators: The volume operator

One of those operators that are implemented on $\mathcal{H}_{\text{kin}}$ is the volume operator and one can rather directly see that it will turn out to be a function of the basic operators introduced right before: Starting with the classical volume of a region R,

$$V(R) = \int_R \mathrm{d}^3x \sqrt{|\det q|} = \int_R \mathrm{d}^3x \sqrt{|\det E|}, \tag{2.102}$$

we see that it depends on the electric fields E. Proceeding towards the operator equivalent, there exist two versions in the literature: one by Rovelli & Smolin [87] and one by Ashtekar & Lewandowski [88]. What they do share is the vertex-wise composition

$$\hat{\mathrm{V}} := \sum_{v \in V(R)} \hat{\mathrm{V}}_v, \tag{2.103}$$

where the sum considers all vertices v that lie in the region R. The vertex-wise evaluation of the volume then differs in three aspects that turn out to make a difference. While

Rovelli–Smolin [87] constructed

$$\hat{\mathrm{V}}_{\mathrm{RS}} \coloneqq \kappa_{\mathrm{V,RS}} \sum_{e_I \cap e_J \cap e_K = v} \sqrt{\left| \epsilon^{ijk} \hat{J}_i^{(v,e_I)} \hat{J}_j^{(v,e_J)} \hat{J}_k^{(v,e_K)} \right|}, \tag{2.104}$$

Ashtekar–Lewandowski [88] obtained

$$\hat{\mathrm{V}}_{\mathrm{AL}} \coloneqq \kappa_{\mathrm{V,AL}} \sqrt{\left| \sum_{e_I \cap e_J \cap e_K = v} \epsilon^{ijk} \epsilon(e_I, e_J, e_K) \hat{J}_i^{(v,e_I)} \hat{J}_j^{(v,e_J)} \hat{J}_k^{(v,e_K)} \right|}. \tag{2.105}$$

First, they rely on two different but equally justified regularisation constants $\kappa_{\mathrm{V,RS}}$ and $\kappa_{\mathrm{V,AL}}$. Secondly, while the Rovelli–Smolin volume adds up the square roots of triples of the $\hat{J}_i^{(v,e)}$ operator, the Ashtekar–Lewandowski volume considers the square root of the sum of these triples. And lastly, Ashtekar–Lewandowski included $\epsilon(e_I, e_J, e_K)$, which takes into account how the three edges are oriented. This inclusion of the edges' orientation yields different results when it comes, for example, to the question of zero-volume-states: When all three edges lie in one plane, the resulting contribution of that triple within the sum is zero — and so does the contribution for arbitrarily valent vertices if all edges are planar.

It was then [89, 90] who considered the dynamics of the theory as a consistency check, using a reformulation of the Hamiltonian constraint by means of Thiemann's identity (confer (2.73) & (2.115) in the next Subsection 2.4.4). They then found that the Ashtekar–Lewandowski volume is to be preferred and we will henceforth use

$$\hat{\mathrm{V}} = {\ell_{\mathrm{P}}}^3 \sum_{v \in V(R)} \sqrt{\left| \frac{1}{48} \sum_{e_I \cap e_J \cap e_K = v} \epsilon^{ijk} \epsilon(e_I, e_J, e_K) \hat{J}_i^{(v,e_I)} \hat{J}_j^{(v,e_J)} \hat{J}_k^{(v,e_K)} \right|} \tag{2.106}$$

$$\eqqcolon {\ell_{\mathrm{P}}}^3 \sum_{v \in V(R)} \sqrt{\left| \hat{\mathrm{Q}}_v \right|} \tag{2.107}$$

for the volume operator. There are a number of reasons why this operator — describing an allegedly intuitive geometrical observable — is in fact not as trivial as one would assume and, what is more, of wide-ranging importance too:

※ First of all, despite the volume being a very much graspable quantity, the calculation of its spectrum turns out to be everything but palpable. While it is straightforward to calculate matrix elements of the operator $\hat{\mathrm{Q}}_v$ — it is just the successive action of three different right-invariant vector fields —, the square root of it that is the volume operator makes the analytical determination of the spectrum of the volume unfeasible so far. Yet, much progress was made by Brunnemann & Thiemann [91] and Brunnemann & Rideout [92–94]. First, [91] simplified the closed formula for matrix elements of the volume operator derived by Thiemann in [95]. This then allowed [92–94] to tackle numerical computations of matrix elements of the volume operator for vertices of valence up to 7 (the 4-vertex was already covered in [91]).

※ Another interesting and counter-intuitive, or at least nonclassical aspect of the volume operator is its spectrum being purely discrete [95–98]. We note that discreteness of the spectrum was also shown for the Rovelli–Smolin volume operator by De Pietri & Rovelli in [99]. This discreteness, however, is in multiples of the Planck volume ${\ell_{\mathrm{P}}}^3$ and therefore experimentally out of reach by state-of-the-art methods.

※ The volume operator and its spectrum also provides a starting point for asking the question of singularity avoidance. As this is one of the main aspects of the work at hand, only a little spoiler will be presented here. Seminal work in the field of loop quantum cosmology (more details on this to follow, too) motivate that the initial Big Bang singularity may in fact have to be replaced by a so-called Big Bounce [41–45]. It is of no surprise that the analogue of the volume operator in loop quantum cosmology plays a crucial role in these kind of considerations and hence, the class of operators one faces during these examinations does indeed include this volume operator. That this is via fractional powers of it makes the computations even more evolved.

※ And lastly, the importance of the volume operator is not just the fact that the volume is a physically intuitive and widely used observable. It is furthermore of uttermost importance for the theoretical footing of loop quantum gravity itself: The quantisation of the Hamiltonian constraint (2.73) was snookered for a long time due to the involved factor ${}^1\!/\!\sqrt{|\det{}^{(\beta_{\mathrm{BI}})}E|}$. It is only for a novel identity Thomas Thiemann introduced in [35] that progress was possible. This identity, as we will see in Subsection 2.4.4, links the inverse volume ${}^1\!/\!\sqrt{|\det{}^{(\beta_{\mathrm{BI}})}E|}$ with the Poisson bracket of the connection and the volume functional — leading upon quantisation to a commutator including the volume operator. This is how the volume operator becomes a crucial ingredient for the whole quantisation process and for progressing towards the dynamics of the theory.

2.4.3 The Gauß and diffeomorphism constraints

Before elaborating on the quantisation of the Hamiltonian constraint, we briefly cover the Gauß and the diffeomorphism constraints, whose smeared versions read

$$G(\Lambda) = \int_\Sigma (\mathcal{D}_a\, E_i^a)\Lambda^i \,\mathrm{d}^3x \quad \text{and} \tag{2.108}$$

$$D\left(\vec{N}\right) = \int_\Sigma F^i_{ab} E^b_i N^a \,\mathrm{d}^3x. \tag{2.109}$$

We keep the discussion of their quantisation rather short and refer to [83] for a more detailed introduction as well as [11, Chapter 9] for a comprehensive discourse.

When it comes to the Gauß constraint, one can also spare oneself its quantisation and solve it classically, proceeding then with gauge-invariant states. However, if one wishes to quantise it nevertheless, the procedure is quite straightforward (cf. e.g. [83, Subsection 3.3.1]) and one ultimately arrives at

$$\hat{G}(\Lambda)T_\gamma(A) = \frac{\mathrm{i}\beta{\ell_\mathrm{P}}^2}{2} \sum_{v\in V(\gamma)} \Lambda^i(v) \left(\sum_{e\in E(\gamma)\colon\, s(e)=v} \hat{X}_i^{(e)} - \sum_{e\in E(\gamma)\colon\, f(e)=v} {}^{(L)}\hat{X}_i^{(e)} \right) T_\gamma(A), \tag{2.110}$$

where $s(e)$ and $f(e)$ denote the starting and ending (final) point of the edge e, respectively. The space $\mathcal{H}^\mathrm{G}$ of solutions to the Gauß constraint is then composed of all those cylindrical functions that result in a vanishing action of $\hat{G}$ — i.e. those states for which the combined overall angular momentum of all ingoing edges ($f(e) = v$) equals that of all outgoing edges ($s(e) = v$) on all vertices v of the graph γ.

The quantisation of the diffeomorphism constraints turns out to be more evolved and one typically draws on the so-called *refined algebraic quantisation*, first applied to the diffeomorphism constraints by Ashtekar, Lewandowski, Marolf, Mourão and Thiemann in [34] and further examined by Giulini and Marolf in [100, 101]. The reason for this extra effort is that if you want to quantise the diffeomorphism constraint, it turns out that the result will not live in $\mathcal{H}_\mathrm{kin}$ and finite diffeomorphisms do not even act in a weakly continuous fashion [83]. However, this situation is surely not too special as also in standard quantum mechanics situations like these exist [102]: Having a particle subject to the constraint of vanishing momentum, e.g., yields non-normalisable solutions that therefore are not element of $\mathcal{H}_{\text{kin}}^{(\text{QM})} = L^2(\mathbb{R}^3)$. The procedure one can then make use of in this case are the so-called rigged Hilbert spaces and that mechanism is also used for finding solutions to the diffeomorphism constraint here. The rigged Hilbert spaces in the quantum mechanical framework read $\mathcal{S} \subset \mathcal{H}_{\text{kin}}^{(\text{QM})} \subset \mathcal{S}^*$, where $\mathcal{S}$ is the Schwartz space of smooth (Schwartz) functions with its dual $\mathcal{S}^*$ being the space of (tempered) distributions, and solutions to the constraint of vanishing momentum live in $\mathcal{S}^*$. For what we face in loop quantum gravity, the rigged Hilbert spaces are $\text{Cyl} \subset \mathcal{H}_{\text{kin}} \subset \text{Cyl}^*$, where Cyl is the space of (smooth) cylindrical functions. Finding solutions to the diffeomorphism constraint is then done by so-called *group averaging* — see, e.g., [103] for an overview. Following [102],[7] this can be performed in two steps, starting by averaging with respect to symmetries $\varphi \in \text{Sym}(\gamma)$ of the underlying graph γ. This results in the projection $\hat{P}_{\text{Sym}(\gamma)}$ onto the graph-symmetry-invariant subspace:

$$\hat{P}_{\text{Sym}(\gamma)}\Psi_\gamma := \frac{1}{N_\gamma} \sum_{\varphi \in \text{Sym}(\gamma)} \varphi^* \Psi_\gamma, \tag{2.111}$$

where N_γ is the size of $\text{Sym}(\gamma)$. However, the follow-up second step consists of averaging over all those diffeomorphisms that translate the underlying graph and this will now not lead to a mere projection, but a map $\eta\colon \text{Cyl} \to \text{Cyl}^*, \Psi \mapsto (\eta(\Psi)|$ instead. Via the inner product $\langle\, .\, , .\, \rangle$ on $\mathcal{H}_{\text{kin}}$, the diffeomorphism invariant action on elements of Cyl is obtained:

$$(\eta(\Psi_\gamma)|\Phi_{\gamma'}\rangle = \sum_{\varphi \in \text{Diff}/\text{Sym}(\gamma)} \langle \varphi^* \hat{P}_{\text{Sym}(\gamma)}\Psi_\gamma, \Phi_{\gamma'}\rangle \quad \text{with} \tag{2.112}$$

$$(\eta(\Psi_\gamma)|\varphi^*\Phi_{\gamma'}\rangle = (\eta(\Psi_\gamma)|\Phi_{\gamma'}\rangle \quad \forall \text{ diffeomorphisms } \varphi. \tag{2.113}$$

If we now only consider those elements of Cyl as input of η that are also solutions to the Gauß constraint (i.e. lie in $\mathcal{H}^{\text{G}}$), we end up with

$$\text{Cyl}^*_{\text{inv}} := \eta\big(\text{Cyl} \cap \mathcal{H}^{\text{G}}\big) \tag{2.114}$$

as the space of solutions to both kinematical constraints — the Gauß and the diffeomorphism constraints.

[7] We also refer to this reference for all the details.

2.4.4 The Hamiltonian constraint

The quantisation of the Hamiltonian constraint will directly affirm the importance of the volume operator discussed in the pre-previous subsection and is therefore the next step. However, with even a nearly comprehensive treatment of this topic being beyond the scope of this introduction into loop quantum gravity, only a condensed overview will be presented that, hopefully, still manages to get the main ideas and important parts across. The interested reader will find an exhaustive treatise in [11, Chapter 10] and a more concise introduction in [83].

While the Hamiltonian constraint is of most importance when it comes to the dynamics of the theory, it is also the constraint that needs the most effort to quantise. With its current form[8]

$$H = \big[\beta_{\mathrm{BI}}^2\, F^i_{ab} - \big(\beta_{\mathrm{BI}}^2 + 1\big)\epsilon^i{}_{jk} K^j_a K^k_b\big] \frac{\epsilon_i{}^{lm} E^a_l E^b_m}{\sqrt{\det q}} = 0 \tag{2.73}$$

containing the inverse of the root of the determinant of the electric fields, i.e. a non-polynomial dependency on a canonical variable, there was not much progress in quantising this expression for some time. A novel quantisation procedure by Thiemann [35, 104–106] then introduced two crucial formulae that allowed for drastic simplifications of the expression above. These two identities read

$$\frac{\epsilon^{ilm} E^a_l E^b_m}{\sqrt{\det q}} = \frac{4}{\kappa}\epsilon^{abc}\big\{V, A^i_c\big\} \quad \text{and} \tag{2.115}$$

$$K^i_a = \frac{2}{\kappa}\big\{\overline{K}, A^i_a\big\}. \tag{2.116}$$

Therein, besides the volume V of a region R, we used

$$\overline{K} := \int\limits_\Sigma \mathrm{d}^3x E^a_i K^i_a. \tag{2.117}$$

At this stage, it is a common practice to split up the Hamiltonian constraint after a previous reformulation that also reflects the correct dimensionality via κ:

$$H(x) = \frac{4}{\kappa\sqrt{\det q}}\,\mathrm{tr}\big([K_a, K_b]\big[E^a, E^b\big]\big) - \frac{2}{\kappa\sqrt{\det q}}\,\mathrm{tr}\big(F_{ab}\big[E^a, E^b\big]\big) \tag{2.118}$$

[8]Note that we dropped the prefix $^{(\beta_{\mathrm{BI}})}$ for the variables and then used $|\det E| = \det q$.

$$=: H_{\text{lor}}(x) - H_{\text{eucl}}(x) \tag{2.119}$$

where H_{eucl} is referred to as the Euclidean part and H_{lor} as the Lorentzian part (this terminology will be used frequently when discussing the Gowdy model in Part II). Recapitulate that we used the convention $\tau_i = -\mathrm{i}\sigma_i$. With the two *Thiemann identities* (2.115) and (2.116), the smeared parts of the Hamiltonian constraint can be rewritten according to

$$H_{\text{lor}}(N) = -8\left(\frac{2}{\kappa}\right)^4 \int_\Sigma N \operatorname{tr}\big(\{A,\overline{K}\} \wedge \{A,\overline{K}\} \wedge \{A,V\}\big) \quad \text{and} \tag{2.120}$$

$$H_{\text{eucl}}(N) = -2\left(\frac{2}{\kappa}\right)^2 \int_\Sigma N \operatorname{tr}(F \wedge \{A,V\}), \tag{2.121}$$

which is a suitable starting point for their quantisation.

For this, we introduce a decomposition $T_\epsilon(\Sigma)$ of Σ into tetrahedra $\triangle$, such that $\bigcup_{T_\epsilon(\Sigma)} \triangle = \Sigma$. This is done including a parameter ϵ that corresponds to the size of the tetrahedra in such a way that the volume of the tetrahedra vanishes for $\epsilon \to 0$. Placing a vertex $v(\triangle)$ at the apex of a tetrahedron (or any corner really), the tetrahedron itself can be defined by three edges $e_I(\triangle)$ starting at that vertex. For the edges of the base, we introduce arcs $a_{IJ}(\triangle)$ that go from the endpoint of $e_I(\triangle)$ to that of $e_J(\triangle)$. With those, we can define loops $\alpha_{IJ}(\triangle)$ around the lateral faces of the tetrahedron (defined by one edge of the base and the vertex on the apex): $\alpha_{IJ}(\triangle) := e_I(\triangle) \circ a_{IJ}(\triangle) \circ e_J(\triangle)^{-1}$. Figure 2.4 illustrates these geometrical quantities exemplarily. Using the positive parameter $\epsilon < 1$ for a rescaling of the edges according to $e(t) \mapsto e(\epsilon \cdot t)$, we can expand the holonomies along edges and loops,

$$h_e(\epsilon) = \mathbb{1}_{\text{SU}(2)} + \epsilon \dot{e}^a(0) A_a^i(v) \frac{\tau_i}{2} + \mathcal{O}\big(\epsilon^2\big) \quad \text{and} \tag{2.122}$$

$$h_{\alpha_{e,e'}}(\epsilon) = \mathbb{1}_{\text{SU}(2)} + \epsilon^2 \dot{e}^a(0) \dot{e}'^b(0) F_{ab}^i(v) \frac{\tau_i}{2} + \mathcal{O}\big(\epsilon^3\big), \tag{2.123}$$

and then use these to replace the Lorentzian and Euclidean parts of the integrated Hamiltonian constraint by Riemann sum equivalents [11]:

$$H_{\text{lor}}^\epsilon(N) = \frac{8}{3}\left(\frac{2}{\kappa}\right)^4 \sum_{\triangle \in T_\epsilon(\Sigma)} \epsilon^{IJK} N(v(\triangle)) \operatorname{tr}\Big(h_{e_I(\triangle)} \Big\{h_{e_I(\triangle)}{}^{-1}, \overline{K}\Big\} \cdot$$

$$\cdot\, h_{e_J(\triangle)}\Big\{h_{e_J(\triangle)}{}^{-1},\overline{K}\Big\}h_{e_K(\triangle)}\Big\{h_{e_K(\triangle)}{}^{-1},V\Big(R_{v(\triangle)}\Big)\Big\}\Big) \quad \text{and} \tag{2.124}$$

$$H^{\epsilon}_{\text{eucl}}(N)=\frac{2}{3}\left(\frac{2}{\kappa}\right)^2\sum_{\triangle\in T_\epsilon(\Sigma)}N(v(\triangle))\epsilon^{IJK}\,\text{tr}\Big(h_{\alpha_{IJ}(\triangle)}h_{e_K(\triangle)}\Big\{h_{e_K(\triangle)}{}^{-1},V\Big(R_{v(\triangle)}\Big)\Big\}\Big). \tag{2.125}$$

Therein, $V\Big(R_{v(\triangle)}\Big)$ describes the volume of a region $R_{v(\triangle)}$ that stands for the proximity of the vertex $v(\triangle)$. Equation (2.125) therefore is in a form that we can already quantise via multiplication operators for the holonomies, (2.94), and the volume operator of (2.106). Lastly, Poisson brackets are replaced by commutators divided by $\mathrm{i}\hbar$: $\{.,.\}\mapsto\frac{1}{\mathrm{i}\hbar}[.,.]$. For the Lorentzian part H_{lor}, however, we still need a way to quantise $\overline{K}$. Via another classical identity, namely

$$\overline{K}=-\{H_{\text{eucl}}(N=1),V\}, \tag{2.126}$$

we can use the previously obtained quantised version of the Euclidean part of the Hamiltonian constraint, together with the volume operator, to obtain the quantised version of the Lorentzian part of the Hamiltonian constraint.

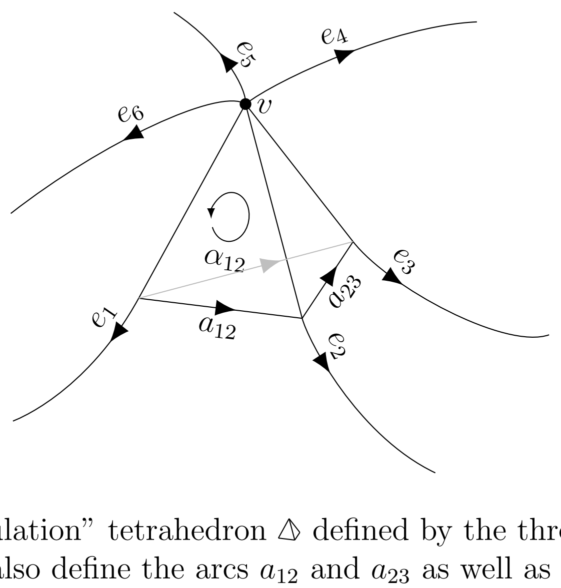


Figure 2.4: A "triangulation" tetrahedron $\triangle$ defined by the three edges $e_{1,2,3}$ that leave vertex v and which also define the arcs a_{12} and a_{23} as well as the loop α_{12} around the face set by a_{12} and v

Ultimately, the action of these operators is understood to have the regularised operator act first, have then the regularisation parameter sent to zero,

$$\hat{H}T_\gamma = \lim_{\epsilon\to 0} H^\epsilon T_\gamma, \tag{2.127}$$

and lastly ensure that the obtained expression is well-defined.

This shows how a quantisation of the Hamiltonian constraint can be achieved. The procedure above, however, yields a Hamiltonian constraint operator that is *graph-changing*: While the three edges leaving the apex of the tetrahedron are per definition (parts of) edges of the underlying graph, the arcs a_{IJ} connecting such edges along the base of the tetrahedron consequently are indeed not. Therefore, every time a holonomy operator along such an arc acts on the graph, this arc is attached to the graph and thereby the graph is changed. In (2.125) above, this happens for the operator representing $h_{\alpha_{IJ}(\triangle)}$, as the loop $\alpha_{IJ}(\triangle)$ along $e_I(\triangle)$ and $e_J(\triangle)^{-1}$ is closed via the arc $a_{IJ}(\triangle)$ — confer Figure 2.4. This behaviour of altering the graph was a crucial aspect of the Hamiltonian constraint operator when Thiemann showed in [104] that it is anomaly free in the sense that the commutator of two Hamiltonian constraints vanishes for diffeomorphism-invariant states. To avoid this addition of new edges, so-called minimal loops [107] can be used during the quantisation. These minimal loops — leaving and entering a vertex of the graph — are exclusively defined via existing edges and of minimal length by means of the number of edges that constitute the loop and hence, a quantisation based on these loops will yield a graph-preserving action.

2.5 Reduced phase space quantisation

The treatment of the Gowdy model in Chapter II will be based on the reduced phase space quantisation, which will be outlined in this section. As introduced before, the name has its origin in the different order of quantising and considering constraints: (some) constraints will be solved already on the classical level and then, on this partially *reduced phase space*, the theory is quantised. We will see that this approach, if applicable to the setup of interest, has the advantage that one obtains a physical Hamiltonian en passant and therefore circumvents the inherent *problem of time* of general relativity.

A key framework within the reduced phase space quantisation (and obtaining a physical time evolution in general relativity) is the so-called *relational formalism* that was introduced by Rovelli in a series of publications [108–111] and later extended by Dittrich [112, 113] and Thiemann [114, 115]. For an introduction, see for example [116] and for an exhaustive treatment [11], while we follow closely [61].

The problem the relational formalism aims to tackle is referred to as the *problem of time* in general relativity: The canonical Hamiltonian of general relativity is built entirely from constraints — cf. (2.31) —, so using this Hamiltonian, which vanishes when all the constraint are fulfilled, for describing the dynamics of observables or states yields a static theory in the quantum theory without any temporal evolution. Experiencing that this is in fact not the case in reality, it is necessary to find out how the dynamics can be described instead.

As we will see, it turns out that in certain models this can be done in a way that looks quite familiar:

$$\frac{\partial \mathcal{O}_f(\tau,\sigma)}{\partial \tau} = \{\mathcal{O}_f(\tau,\sigma), H_{\text{phys}}\}. \tag{2.128}$$

The only difference being the new quantities $\mathcal{O}_f(\tau,\sigma)$ and some — to be further specified — physical Hamiltonian H_{phys}. Now, the reason why it is called the relational formalism is due to reference fields T^I that are introduced, to wit: one per constraint. The *observable* $\mathcal{O}_f(\tau,\sigma)$ of a phase space function f then tells the value f takes when these *clocks* T^I take the values τ^I. To use the intuitive split of space and time, the clock T^0 linked to the Hamiltonian constraint C_0 is usually referred to as $T := T^0$, taking the value $\tau := \tau^0$ at evaluation. The remaining reference fields $T^{I\neq 0}$ are then relabelled as $S^I := T^{I\neq 0}$, taking values $\sigma^i := \tau^{i\neq 0}$, and the set σ of all σ^i can be used to coordinatise the so-called dust manifold $\mathcal{S}$.

We now introduce the procedure for the general case and then return to the special scenario of general relativity as announced above. Facing a system with a set of constraints C_I, the first step of the construction of the observable $\mathcal{O}_f$ consists of weakly *abelianising* the constraints [112]: The constraints C_I do not necessarily commute, $\{C_I, C^J\} \neq 0$, but we can proceed to a new set of constraints that indeed does. With the introduction of

$$M_I^J := \{C_I, T^J\}, \tag{2.129}$$

we define a new set of constraints via

$$C'_I := \left(M^{-1}\right)_I^J C_J. \tag{2.130}$$

This, of course, implies that we need to use such T^J for which M_I^J is invertible. The new set of constraints now has the advantage that

$$\left\{C'_I, T^J\right\} \approx \delta_I^J. \tag{2.131}$$

Therein, $\approx$ symbolises that the equation holds at least on the *constraint hypersurface* $\overline{\mathcal{M}}$, i.e. when all constraints are fulfilled: $\overline{\mathcal{M}} = \{m \in \mathcal{M} \colon C_I(m) = 0 \; \forall \, C_I\}$. We can then state the Hamiltonian vector field of the linear combination

$$C_\beta := \beta^I C'_I \;, \quad \beta^I \in \mathbb{R}, \tag{2.132}$$

of the constraints C'_I as

$$X_\beta = \beta^I X_I, \tag{2.133}$$

where the Hamiltonian vector field X_I of a single constraint C'_I reads

$$X_I := \{C'_I, \cdot\}. \tag{2.134}$$

With X_β, we can as a next step define the gauge flow $\alpha_\beta(f)$ of a phase space function f [112, 117]:

$$\alpha_\beta(f) := \exp(X_\beta) f. \tag{2.135}$$

This allows us to move f along the flow of the linear combination C_β of the abelianised constraints C'_I. But, of course, we want to do this in a controlled way, in particular in a way which we can associate with a temporal evolution. This can be achieved by considering the gauge flow of the reference fields T^I simultaneously. As it was already stated above, the relational framework describes the evolution of observables with respect to those reference fields. Accordingly, we evaluate the gauge flow of the respective phase space function with respect to the gauge flow of the reference fields and get

$$\mathcal{O}_f(\tau) := \alpha_\beta(f)\big|_{\alpha_\beta(\{T^I\}) = \{\tau^I\}} \tag{2.136}$$

as the value f takes when the reference fields T^I take the values τ^I.

There are now some remarks to be made, where the last one also specifies the scenario this work is about and motivates the structure of the initial evolution equation (2.128):

※ First, equation (2.135) contains the exponential and hence products of X_β, which in turn is a linear combination of the X_I. Therefore, the order of the respective factors X_I in (2.135) matters — in general. This is the reason why the new abelianised set of constraints C'_I was used as these lead to *weakly commuting* Hamiltonian vector fields X_I. Similar to before, the property of two variables weakly commuting means that they do commute when restricted to the constraint hypersurface $\overline{\mathcal{M}}$.

※ Furthermore, the observables $\mathcal{O}_f$ are *weak Dirac observables*, which means that they weakly commute with the constraints:

$$\{\mathcal{O}_f(\tau), C_I\} \approx 0 \; \forall \, C_I. \tag{2.137}$$

So they really are gauge invariant extensions of gauge variant phase space functions and qualify for physically observable quantities.

※ When working with the observables $\mathcal{O}_f$, there are a couple of identities that make calculations much easier. The most important ones are

$$\mathcal{O}_f(\tau) + \mathcal{O}_{f'}(\tau) = \mathcal{O}_{f+f'}(\tau), \tag{2.138}$$

$$\mathcal{O}_f(\tau) \cdot \mathcal{O}_{f'}(\tau) \approx \mathcal{O}_{f \cdot f'}(\tau), \tag{2.139}$$

$$\{\mathcal{O}_f(\tau), \mathcal{O}_{f'}(\tau)\} \approx \mathcal{O}_{\{f,f'\}^*}(\tau) \text{ and} \tag{2.140}$$

$$\mathcal{O}_{f(A,E,T^I,P_I)}(\tau) \approx f\big(\mathcal{O}_A(\tau), \mathcal{O}_E(\tau), \mathcal{O}_{T^I}(\tau) = \tau^I, \mathcal{O}_{P_I}(\tau)\big). \tag{2.141}$$

In the second last equation, $\{\,\cdot\,,\,\cdot\,\}^*$ denotes the Dirac bracket, which is an extension of the Poisson bracket and necessary when facing a system with second class constraints. For the present case of having both a set of gauge fixing conditions $\mathcal{G}^I := T^I - \tau^I =: C_{2I}$ and one of second class constraints $C_I =: C_{1I}$, all collected in C_μ, the Dirac bracket reads [114]

$$\{f, f'\}^* = \{f, f'\} - \{f, C_\mu\} \mathcal{M}^{\mu\nu} \{C_\nu, f'\}, \tag{2.142}$$

with the coupling $\mathcal{M}^{\mu\nu} := \{C_\mu, C_\nu\}$.

※ Last but not least, going back to the case of general relativity, the physical Hamiltonian H_{phys} that enters equation (2.128) and creates the evolution of the observables needs to be defined. The steps to perform from this point onwards depend heavily on the kind of reference fields one introduces and on the general model considered. For a broad overview over the different kinds of reference fields and their treatment, see for example [118]. We will now exemplarily sketch the path similar to the upcoming investigations of Chapter II. There, introducing Gaussian dust [119] as the reference fields T^I allows for a simplified description of the constraints. For the total Hamiltonian constraint $H = C_0$ consisting of all degrees of freedom, including those of the reference fields, this new form reads

$$H = C_0 = P + h(A, E), \tag{2.143}$$

where P is the canonically conjugate of $T = T^0$. This form is referred to as a *deparametrised form* due to the fact that we can write the Hamiltonian constraint in a form that is linear in P and where h does not depend on T. The part $h(A, E)$ independent of the reference field variables (T, P) can then be used to define the time-independent[9] physical Hamiltonian that describes the temporal evolution of the observables according to (2.128) [115]:

$$H_{\text{phys}} \coloneqq \int_{\mathcal{S}} \mathcal{O}_h \, \mathrm{d}\sigma. \tag{2.144}$$

Having a system in deparametrised form also simplifies several formulae we stated before. By definition, $M_I^J = \{C_I, T^J\} = \delta_I^J$ holds, which implies $C_I' = C_I$. Note that the diffeomorphism constraints can not be deparametrised as the Hamiltonian constraint. However, one can achieve getting

$$C_{I\neq 0} = P_I + h_I\big(A, E, S^I\big) \tag{2.145}$$

and the fact that it still only depends linearly on P_I suffices for $M_I^J = \delta_I^J$. Additionally, many of the weak equations become strong ones for deparametrised systems — like $\{C_I, C_J\} = 0$ and therefore $[X_I, X_J] = 0$, too. Hence, performing the weak abelianisation is not necessary when working with a deparametrised theory.

Finally, when it comes to the follow-up quantisation, deparametrised theories share the feature that the observable algebra turns out to be isomorphic to a subset of the kinematical algebra. With that, the representation used for the kinematical Hilbert space in the case of the Dirac quantisation procedure becomes a representation directly accessing the physical Hilbert space. Thus, we can implement the Ashtekar–Lewandowski representa-

[9] If h still depends on T, the resulting physical Hamiltonian is in general time-dependent.

tion here, $\mathcal{H}_{\text{phys}} = L^2(\overline{\mathcal{A}}, \mathrm{d}\mu_{\text{AL}})$, and choose the spin network functions T_γ as a suitable basis. Note that we did respect the classical symmetries of the system during the reduced phase space quantisation and, accordingly, so should the resulting H_{phys}. However, [34] showed that diffeomorphism invariant operators whose actions alter the underlying graph can not be densely defined on $\mathcal{H}_{\text{kin}}$ — which is why we need to implement the physical Hamiltonian in a graph-preserving manner.

2.6 Algebraic quantum gravity

The last framework we want to outline is the so-called *algebraic quantum gravity*. Introduced in a series of papers by Giesel and Thiemann in [58–61], the name reflects the fact that algebraic quantum gravity considers only one abstract and countably infinite algebraic graph α. This graph is still adapted to the model one studies, so it might be of cubic topology or, as we see later on in Chapter II for a symmetry reduced model, just a one-dimensional line. However, the important part is that this graph will not be changed in its *structure* by the action of any operator and only the charges on the edges and vertices will be modified. As before, representations of SU(2) are associated with all of the graph's edges, but for algebraic quantum gravity also trivial representations can be assigned. So no edges will be removed or added, but trivially 'charged' edges can be charged and, vice versa, previously charged edges may turn into trivially charged ones, thus mimicking the graph-changing behaviour of loop quantum gravity operators. The naming *abstract* graph furthermore does indeed mean that the graph, its edges and vertices, do have no geometrical or even physical meaning — at least until an embedding into a manifold may be chosen. The Hilbert space structure then is the infinite tensor product of the edges' Hilbert spaces $L_2(\mathrm{SU}(2), \mathrm{d}\mu_{\mathrm{H}})$, where the holonomy and flux operators act as edge-wise multiplication and differentiation operators, respectively, and also the inner product is just the edge-wise product of the respective inner products per edge. This infinite tensor product of Hilbert spaces was introduced by von Neumann in [120] and first implemented in the framework of loop quantum gravity by Thiemann and Winkler in [121].

Now, one of the reasons why algebraic quantum gravity was introduced has to do with the semiclassical realm of quantised general relativity, where it is important to be able to retrieve classical general relativity in some limit. It turns out that this framework allows to introduce such a semiclassical analysis [59], even including computable semiclassical perturbation theory with error control [60].

This finishes the introduction of theoretical frameworks in the realm of quantum gravity that are important for the upcoming chapters. The next section treats the last tool that we need for our considerations of Part III: semiclassical states, also referred to as coherent states.

2.7 Coherent states

The concept of quantum mechanical states that are *as close to classical states as possible* is well-known from quantum mechanics, where they are typically called *coherent states*. They also go by the name *semiclassical states*, stemming from their defining property. Semiclassical states were first constructed by Schrödinger in 1926, when he was looking for those states of the quantum mechanical harmonic oscillator that behave like states of the classical one in order to find the "stetige Übergang von der Mikro- zur Makromechanik" [122] — i.e. the steady transition from micro- to macro-mechanics. That coherent states then became mostly known for their application in quantum optics and quantum electrodynamics is of no surprise, are these fields working on the link between the classical and the quantum world. Most progress in the theoretical direction is among others due to Klauder, Sudarshan and Glauber (see [123–125], to state the main articles for all three of them). From the experimental side, the work of Hanbury Brown and Twiss [126, 127] was a starting point to investigate different types of light regarding coherence, followed by many important contributions from others, too. They thereby opened the door for a new kind of (astronomical) interferometry by using it to measure the angular diameter of Sirius [128].

We already motivated why the semiclassical realm is important for quantum gravity — it should recover classical relativity as a limit. For having a tool at hand which can provide the link between quantum and general relativity, coherent states were studied also in this field. Based on work of Ashtekar, Lewandowski, Marolf, Mourão and Thiemann in [129] — who in turn drew upon work of Hall [130], Segal [131] and Bargmann [132] — so-called *complexifier coherent states* were introduced by Thiemann in [133]. This approach has constantly been further developed [62, 121, 134–137] and became the state-of-the-art framework for coherent states in loop quantum gravity. We note that [62] showed that other coherent states constructed for quantum gravity, Varadarajan's "polymer-like" coherent states [138–140], are in fact also part of the class of complexifier coherent states and so are the coherent states of the quantum mechanical oscillator [11, Subsection 11.2.2].

Now, what are the requirements in order to classify a state as a semiclassical or coherent one? Thiemann uses a two-fold definition in [11]: While one collects three properties that specify what "semiclassical" is supposed to mean (Definition 11.2.1. therein), the other one contains four more mathematically necessary ones (Definition 11.2.2.). We loosely recite them in the following list, where the first three specify "semiclassicality" and the remaining four are the aforementioned mathematical necessities:

1. The expectation value $\langle\Psi|\hat{O}|\Psi\rangle$ of operators in the semiclassical limit are close to the classical expectation value O of the associated classical observable:
$$\left|\frac{\langle\Psi,\hat{O}\Psi\rangle}{O}-1\right|\ll 1 \tag{2.146}$$

2. The expectation value of the commutator of two operators in the semiclassical limit are close to the classical expectation value of the Poisson bracket of the associated classical observables times i$\hbar$:
$$\left|\frac{\langle\Psi,\left[\hat{O},\hat{O}'\right]\Psi\rangle}{\mathrm{i}\hbar\{O,O'\}}-1\right|\ll 1 \tag{2.147}$$

3. The fluctuations of the expectation value of operators in the semiclassical limit are small:
$$\left|\frac{\langle\Psi,\hat{O}^2\Psi\rangle}{\langle\Psi,\hat{O}\Psi\rangle^2}-1\right|\ll 1 \tag{2.148}$$

4. Overcompleteness: The coherent states allow for a resolution of unity:
$$\mathbb{1}=\int \mathrm{d}\mu\Psi\langle\Psi,\cdot\rangle \tag{2.149}$$

5. The coherent states are eigenstates of an operator $\hat{a}$, typically referred to as the annihilation operator:
$$\hat{a}\Psi=a\Psi \tag{2.150}$$

6. Minimal uncertainty: The coherent states fulfil the Heisenberg uncertainty relation exactly, i.e. with the equal sign:

$$\langle \Psi, (\hat{x} - \langle \Psi, \hat{x}\Psi \rangle)^2 \Psi \rangle = \frac{1}{2} |\langle \Psi, [\hat{x}, \hat{p}] \Psi \rangle| = \langle \Psi, (\hat{p} - \langle \Psi, \hat{p}\Psi \rangle)^2 \Psi \rangle \tag{2.151}$$

7. Peakedness: The coherent states, or rather their overlap functions $|\langle \Psi, \Psi' \rangle|$, are concentrated in a small cell of phase space

It makes a lot of sense to say that the first three do indeed characterise a "semiclassical" state: Expectation values should be as close to the classical ones as possible and fluctuations better be small. It is already noted in [11] that these properties are not entirely independent of each other, as for example (5) leads to (6). Also, one could understand (7) as a semiclassicality-property, too. Nevertheless, this list is certainly appropriate as an overview of necessary characteristics for coherent states.

Now, complexifier coherent states get their name by the so-called *complexifier* that is crucial for their construction. For the quantum harmonic oscillator coherent states, the complexifier (operator) reads [11]

$$\mathcal{C}_{\text{ho}} := \frac{p^2}{2m\omega}, \quad \hat{\mathcal{C}}_{\text{ho}} := \frac{\hat{p}^2}{2m\omega} \tag{2.152}$$

and it can be used to construct the eigenvalue a of the annihilation operator $\hat{a}$ as well as $\hat{a}$ itself:

$$\begin{aligned} a &= \frac{\sqrt{m\omega}x - \frac{\mathrm{i}}{\sqrt{m\omega}}p}{\sqrt{2}} &(2.153)\\ &\equiv \frac{m\omega}{2} \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \{\mathcal{C}_{\text{ho}}, x\}_n \quad \text{and} &(2.154)\\ \hat{a} &= \frac{m\omega}{2} \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \frac{\left[\hat{\mathcal{C}}_{\text{ho}}, \hat{x}\right]_n}{(\mathrm{i}\hbar)^n} &(2.155)\\ &= \frac{m\omega}{2} \mathrm{e}^{-\frac{\hat{\mathcal{C}}_{\text{ho}}}{\hbar}}\, \hat{x}\, \mathrm{e}^{\frac{\hat{\mathcal{C}}_{\text{ho}}}{\hbar}} = \frac{m\omega}{2} \mathrm{e}^{\frac{t}{2}\Delta}\, \hat{x}\, \mathrm{e}^{-\frac{t}{2}\Delta} &(2.156) \end{aligned}$$

Therein, the iterated Poisson bracket $\{\mathcal{C}, x\}_n$ is defined via $\{\mathcal{C}, x\}_0 = x$ and $\{\mathcal{C}, x\}_n = \left\{\mathcal{C}, \{\mathcal{C}, x\}_{n-1}\right\}$ and likewise for the iterated commutator $[.,.]_n$. Additionally, note that

$\hat{p}^2 = -\hbar^2\Delta$ and we defined

$$t := \frac{\hbar}{m\omega} \tag{2.157}$$

as the *classicality parameter* of the quantum harmonic oscillator. For a state $\psi_x(x') = \mathrm{e}^{-\frac{t}{\hbar^2}\hat{C}_{\mathrm{ho}}}\delta_x(x')$, the following eigenvalue equation is at least formally fulfilled, when we regard the δ-distribution as an eigendistribution of $\hat{x}$:

$$\hat{a}\psi_x(x') = \sqrt{\frac{m\omega}{2}}x\psi_x(x'). \tag{2.158}$$

However, we do not yet have $\hat{a}\psi_x = a\psi_x$. To achieve this, we analytically extend the state to the complex plane via $x \mapsto z = x - \frac{\mathrm{i}}{m\omega}p$ and then have indeed $\hat{a}\psi_z = a\psi_z$ for the new states ψ_z that in fact equal the well-known harmonic oscillator coherent states up to a phase.

The construction of the complexifier coherent states for quantum gravity can now be carried over quite straightforwardly. However, note that we just *stated* the complexifier for the quantum harmonic oscillator — there is no rigorous way of constructing one. Definition 2.1 of [62] specifies a complexifier as a

- positive definite,
- almost everywhere smooth function with
- dimension of an action, whose
- Hamiltonian vector field does not vanish anywhere and which
- is at least linear in the momentum variable.

Having chosen a complexifier C, one can continue with the construction procedure. While (x, p) represented position and momentum for the quantum harmonic oscillator before, we now use (q, p), representing the generalised configuration and conjugate momentum variable.[10] We collect them in the tuple $m := (q, p)$ and then build the complex coordinate via

$$Z(m) := \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!}\{C, q\}_n(m). \tag{2.159}$$

[10] Note that we understand these quantities to be smeared appropriately with test functions, thus allowing us to omit any labels.

Note that the requirements for the complexifier above guarantee that we can re-obtain q and p from Z and its complex conjugate $\overline{Z}$. Also, with $\mathcal{C}$ being required to be positive definite, we quantise it as a positive, self-adjoint operator $\hat{\mathcal{C}}$. With this, the generalised annihilation operator can be constructed:

$$\hat{Z} := \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \frac{\left[\hat{\mathcal{C}}, q\right]_n}{(\mathrm{i}\hbar)^n} = \mathrm{e}^{-\frac{\hat{\mathcal{C}}}{\hbar}}\, \hat{q}\, \mathrm{e}^{\frac{\hat{\mathcal{C}}}{\hbar}}, \tag{2.160}$$

where now the fact that the complexifier is of the dimension of an action makes the exponential well-defined. We can now proceed towards the state via the intermediate step

$$\psi_q(q') := \mathrm{e}^{-\frac{\hat{\mathcal{C}}}{\hbar}} \delta_q(q'), \tag{2.161}$$

which we now need to analytically continue to the complex plane. For this, the property of the complexifier to be growing more than linearly in p plays a crucial role as it ensures a hyper-exponential damping necessary for ψ_q to be analytic. We finally obtain

$$\Psi_m(q') := \psi_q(q')\Big|_{q \mapsto Z(m)} = \left(\mathrm{e}^{-\frac{\hat{\mathcal{C}}}{\hbar}} \delta_q\right)(q')\Big|_{q \mapsto Z(m)} \tag{2.162}$$

for the general version of the complexifier coherent states.

For adapting these states to the case of quantum gravity, we refer to [66, Appendix C], as we will work with their form and notation of the coherent states throughout Chapter III. Using connections and fluxes, the coherent states read in general

$$\Psi_m(A') = \left(\mathrm{e}^{-\frac{\hat{\mathcal{C}}}{\hbar}} \delta_A\right)(A')\Big|_{A \mapsto Z(m)}. \tag{2.163}$$

Again, $m = (A(x), E(x))$ denotes the point in phase space the state is peaked around and the complexified connection $Z(m)$ is constructed analogously via (2.159). Now, the δ-distribution we use, $\delta_A(A')$, is the one of the kinematical Hilbert space $\mathcal{H}_{\mathrm{kin}} = L^2\left(\overline{\mathcal{A}}, \mathrm{d}\mu_{\mathrm{AL}}\right)$ with support at A.

During our computations of Chapter III, we will use these kind of states for the gauge group $\mathrm{U}(1)^3$. This is an ansatz widely used in the literature (cf. i.a. [63–66, 134, 135]) and is motivated due to the fact that replacing the actual gauge group $\mathrm{SU}(2)$ by $\mathrm{U}(1)^3$ does not change the outcome qualitatively, but simplifies the calculations drastically for $\mathrm{U}(1)^3$

being abelian — and thus making the $\mathrm{U}(1)^3$ coherent states eigenstates of the volume operator [134, 135]. In the notation of [66], the $\mathrm{U}(1)^3$ coherent state peaked around $m = \big(A^{(0)}(x), E^{(0)}(x)\big)$ reads

$$\Psi_m(A) = \prod_{\substack{e_I \in E(\gamma) \\ i=1,2,3}} \sum_{\{n_I^i\} \in \mathbb{Z}} \mathrm{e}^{-\frac{t}{2}\left(n_I^i\right)^2 + n_I^i p_I^i(m)} \left[\mathrm{e}^{\mathrm{i}\theta_I^i(m)} \mathrm{e}^{-\mathrm{i}\theta_I^i(A)}\right]^{n_I^i}. \tag{2.164}$$

We will describe the $\mathrm{U}(1)^3$ framework more detailed in Chapter III and only briefly explain the above quantities at this stage. Introducing $\mathrm{U}(1)^3$ means equipping all edges e_I of the graph γ with three copies of $\mathrm{U}(1)$. These are labelled by the three charges $n_I^i \in \mathbb{Z}$, $i = 1, 2, 3$. The $\mathrm{U}(1)$-holonomy — whose inverse we find as the above square bracket's second exponential function — reads

$$h_I^i(A) = \mathrm{e}^{\mathrm{i} \int_{e_I} A_a^i(e_I(t))\, \dot{e}_I^a(t)\ \mathrm{d}t} =: \mathrm{e}^{\mathrm{i}\theta_I^i(A)}, \tag{2.165}$$

and its complexified extension is

$$h_I^i(Z(m)) = \mathrm{e}^{p_I^i(m)} h_I^i(A|_m) =: \mathrm{e}^{p_I^i(m)} \mathrm{e}^{\mathrm{i}\theta_I^i(A|_m)}. \tag{2.166}$$

This complexified holonomy contributes the first exponential in the square bracket of the coherent state. The quantity $p_I^i(m)$ therein constitutes the canonically conjugate variable to the holonomy $h_I^i(A)$. Lastly, we note that in contrast to [66], we do not consider the classicality parameter t to be different for the graph's edges, but rather use one t for all of them. This is not a necessary substitution, but keeps the formulae more concise.

We close this introduction of the coherent states with some notes on their limitations.

※ First, these coherent states are kinematical ones, i.e. the action of the constraint operators does not necessarily vanish. But this indeed makes sense: Recapitulating that we want to use these semiclassical states to check whether, e.g., the Hamiltonian has the correct classical limit, such an investigation can not be performed would the action of the Hamiltonian annihilate the coherent state.

※ Second, their dynamical stability is not guaranteed, meaning that an initial coherent state does not automatically evolve in time such that it remains a coherent state. This can be easily motivated if one thinks about the two ways the temporal evolution manifests for coherent states. On the one hand, we can simply evolve a just created coherent state. On the other hand, having started with a coherent state peaked around some $m_0 = \big(A^{(0)}, E^{(0)}\big)$, we can use the classical evolution of the system to determine the phase space point $m(t) = \big(A^{(t)}, E^{(t)}\big)$ around which the state should be peaked later on. Constructing the coherent state according to the complexifier procedure for this future $m(t)$ does not necessarily result in the same state. However, there is new progress in this direction [141].

※ Third, the coherent states are only suitable for determining the semiclassical expectation value of phase space functions whose corresponding operators preserve the underlying graph. When an operator adds a new edge, there is now way the coherent state can 'know' how to approximate the contribution of this edge if it was not already included in its construction. This is one of the reasons why algebraic quantum gravity seems to be a suitable framework for semiclassical investigations as all operators act in a graph preserving manner there.

Part II

Gowdy models

Chapter 3

Motivation

Note that the content of this part, Part II, was already published in [1]. The text of this article has been reused.

Loop quantum gravity provides a framework in which an analogue of the classical Einstein's equations can be formulated in the quantum theory. In the canonical approach, one either considers solving the constraints in the quantum theory in the context of a Dirac quantisation [78] or one solves the constraints already at the classical level by means of constructing suitable Dirac observables and subsequently quantises the physical phase space only. In full loop quantum gravity, both approaches yield quantum Einstein's equations that are very complex and whose general solutions are not known [11–13, 142]. This is not too surprising because already at the classical level the Einstein's equations without further assumptions are highly complex and constructing exact solutions is a very non-trivial task. However, exact solutions can be constructed in simpler setups where additional symmetry assumptions are implemented such as for instance in the context of cosmology or black holes. If we consider symmetry reduction in the context of a quantum gravity theory, one can either symmetry reduce already at the classical level and then quantise or one can quantise full general relativity and afterwards access the symmetry reduced sector in the quantum theory. While the latter strategy is presumably the one that is able to capture more of the quantum nature of the symmetry reduced models [47, 143–145], it is also technically more involved than first symmetry reducing at the classical level and quantising only afterwards.

For this reason, we follow the first approach in this part and consider a symmetry reduction of classical models that experience a Gowdy symmetry [146]. We furthermore specialise to the polarised case where the two commuting Killing vectors are orthogonal. Compared to other symmetry reduced homogeneous models in cosmology, such models similar to spherically symmetric models have the property that they are still a field theory with a non-trivial spatial diffeomorphism constraint and thus are closer to the situation we face in full general relativity. Hence, understanding these models allows to investigate properties of these models that might be absent in the homogeneous cosmological models in general. As we still have to deal with a constrained theory after symmetry reduction, we have again the option to either apply a Dirac or reduced quantisation of the symmetry reduced model where we follow the latter in this work. The quantisation of Gowdy models has been extensively discussed in the existing literature [147–151] starting after Gowdy's seminal paper [146]. Further work in terms of (complex) Ashtekar variables can be found in [152–155]. The quantisation programme could be completed in the context of a gravitational wave quantisation in geometrodynamics in [156], see also [157] for a further extension of this model. A modified quantisation of the model in [156] was later considered in order to ensure that the dynamics is unitary [158–162]. All these models have in common that even if some of them start with Ashtekar variables the final quantum model does not involve a quantisation inspired from loop quantum gravity but considers techniques from geometrodynamics instead after gauge fixing the models. As a consequence, these models fail to resolve the singularity present in the classical Gowdy model. In [163, 164], a loop quantisation of the polarised $\mathbb{T}^3$ Gowdy has been introduced in the framework of a Dirac quantisation. However, due to the complicated form of the constraint operators, the quantisation programme could not be completed for that model. Progress in this directions was obtained using a hybrid quantisation procedure where the polymetric quantisation is applied to the homogeneous sector and a Fock quantisation to the inhomogeneous one [165–167]. A uniqueness result for the chosen Fock quantisation exists [168] if one demands unitary implementation of the dynamics as well as invariance under the group of constant translations on the circle. This approach has turned out to be also useful in the context of cosmological perturbations, see for instance [169–171] and [172] for a recent review on the hybrid quantisation approach.

Because we will apply a reduced phase space quantisation for which we choose Gaussian dust as the reference matter [118, 119], we cannot consider the usual Gowdy solution that is a vacuum solution of Einstein's equations. Spacetimes with Gowdy symmetry coupled to matter have been considered in the literature, see for instance [173] for a coupling to a massless scalar field. For a corresponding quantum model see [174] and [175] for work on Einstein–Vlaslov spacetimes with Gowdy symmetry extending former results for the vacuum case [176, 177]. An introduction to the Einstein–Vlasov system can be found in [178] and references therein. As discussed in [179], dust can be understood as a distributional solution of the Vlasov equation and in this sense can be embedded in these systems. However, the specific characteristic properties of the matter component matter as for instance the results in [180] show where the properties of the spacetimes are different if we couple generic Vlasov matter or dust respectively in the context of finding a global foliation of the spacetime. For the purpose of this work, we consider general relativity coupled to Gaussian dust and then impose a Gowdy symmetry on the total system including the geometric as well as the matter degrees of freedom.

This setup allows us to construct Dirac observables associated with the geometric degrees of freedom in the framework of the relational formalism along the lines of [109, 111–114, 181–183] that play the role of the elementary phase space variables in the reduced phase space. Their dynamics is generated by a so-called physical Hamiltonian whose Hamiltonian density in the Gaussian dust model is just given by the geometric contribution to the Hamiltonian constraint that is itself a Dirac observables and non-vanishing in the physical sector of the model [118, 119]. Further reference matter models as well as their applications in the classical theory can for instance be found in [184–188] and applications in the quantum theory are for example discussed in [44, 61, 118, 189–193]. Dirac observables for vacuum Gowdy spacetimes have for instance also been discussed in [194]. In the context of the relational framework, this approach can be understood as choosing so-called geometrical clocks (or reference fields) constructed from purely geometric degrees of freedom. In contrast, we choose matter clocks in this work instead. As a consequence, we start with additional degrees of freedom compared to [194], where in the end one independent Dirac observables exists, while here we end up with three independent ones. Furthermore, the construction of [194] is based on ADM variables, whereas here we will work with Ashtekar–Barbero variables in order to be able to apply a loop quantisation to the model later on.

Loop quantisations that do not apply a hybrid approach of vacuum polarised $\mathbb{T}^3$ Gowdy spacetimes in the context of a Dirac quantisation have been considered in [164, 195], where the latter model assumes a further rotational symmetry that simplifies the setup compared to [164]. The difference to the work here is that we consider a reduced phase space quantisation in the context of loop quantum gravity (LQG) as well as the algebraic quantum gravity (AQG) framework for the Gaussian dust model. In both cases the physical Hamiltonian needs to be quantised in a graph-preserving manner in order to respect the classical symmetries of the physical Hamiltonian. This yields a different regularisation of the operator compared to the one presented in [164], with in general different properties accordingly. Possible graph-preserving quantisations have been discussed in [196] in the context of spherically symmetric models and have also been mentioned in the final discussion of [164] as possible alternative regularisations. However, since in both works one uses Dirac quantisation with the corresponding constraint algebra in these models, a graph-modifying quantisation is motivated for the same reason we have in full LQG.

Because we quantise the physical Hamiltonian in the AQG framework, a detailed discussion on how Gowdy states can be represented in the AQG framework is needed, allowing to implemented the action of the physical Hamiltonian operator on this class of states properly. The dynamics of the physical states is encoded in a Schrödinger-like equation and finding its generic solution is beyond the scope of this part. Nevertheless, the quantisation programme can be completed in this model here in the sense that the quantum dynamics is formulated at the level of the physical Hilbert space. The purpose of this work is to present how spacetimes with a Gowdy symmetry can be formulated in the AQG framework. The results presented here can be taken as the starting point for deriving effective models directly from the quantum theory because the graph-preserving regularisation chosen here is advantageous if semiclassical computations are to be performed as already existing semiclassical techniques can be directly used and need not be adapted to graph-modifying operators — which is still an open and difficult questions in full generality. As first steps towards applying the model, we compute the explicit form of the Schrödinger-like equation in the AQG framework and discuss a possible ansatz for the solution that can be considered for graph-preserving operators but will not work for graph-modifying ones as used in [164]. We further discuss how such an ansatz can be used to obtain zero volume eigenstates.

Chapter 4

Classical Setup: formulation of the model with polarised $\mathbb{T}^3$ Gowdy symmetry

In this chapter, we briefly review the Gaussian dust model as well as its symmetry reduction to a model having a $\mathbb{T}^3$ Gowdy symmetry.

4.1 Brief review of the classical reduced phase space using Gaussian dust

We aim at quantising the reduced phase space of general relativity formulated in terms of Ashtekar variables and symmetry reduced to the polarised Gowdy model. For this purpose, we choose as a first step some reference matter that we dynamically couple to gravity and that allows us to construct the corresponding elementary Dirac observables in the reduced phase space. For the reference matter we choose the Gaussian dust model [119] that was for instance considered in [118] in the context of loop quantum gravity. Within the Gaussian dust model, one couples eight additional scalar fields to general relativity, leading to a system that involves second class constraints. As shown in [118, 119], after a reduction with respect to the second class constraints one obtains a first class system and next to gravity four additional dust fields — denoted by T and S^j with $j = 1, 2, 3$ — that can be used as reference fields for the Hamiltonian and spatial diffeomorphism constraints respectively. In this model, these constraints take the form

$$C^{\text{tot}} = C + \frac{P - \frac{E^a_j E^b_k \delta^{jk}}{\det(E)} T_{,a} C_b}{\sqrt{1 + \frac{E^a_j E^b_k \delta^{jk}}{\det(E)} T_{,a} T_{,b}}}, \quad C^{\text{tot}}_a = C_a + P T_{,a} + P_j S^j_{,a}.$$

Here, C and C_a denote the gravitational contribution to the total Hamiltonian and spatial diffeomorphism constraints[1] in terms of the Ashtekar variables A^j_a, E^a_j, while P, P_j are the momenta conjugate to T, S^j. Following [118], one solves C^{tot} for P and C^{tot}_a for P_j and then writes down an equivalent set of constraints that now is Abelian. The latter allows to directly apply the known observable map [112, 113, 181] in the framework of the relational formalism [109, 111] and construct the corresponding Dirac observables for the gravitational degrees of freedom denoted as $\mathcal{O}_{A^j_a}$ and $\mathcal{O}_{E^a_j}$. The algebra of the observables is given by

$$\{\mathcal{O}_{A^j_a}(\tau,\sigma), \mathcal{O}_{E^b_k}(\tau,\sigma')\} = \frac{\kappa}{2}\delta^b_a \delta^j_k \delta^{(3)}(\sigma - \sigma'), \tag{4.1}$$

where we use $\kappa := 16\pi G_{\text{Newton}}$.

Using the properties of the observable map as shown in [114], for a phase space function $f(A,E)$ we further have

$$\mathcal{O}_{f(A,E)(\tau,\sigma)} \approx f(\mathcal{O}_A(\tau,\sigma), \ldots, \mathcal{O}_E(\tau,\sigma)), \tag{4.2}$$

where in general only a weak equality holds — i.e. one that only holds on the so-called constraint surface, the hypersurface on which all constraints are fulfilled. Hence, it is sufficient to construct Dirac observables for the elementary geometric phase space variables. To obtain their explicit form, one chooses T as the temporal reference field for the Hamiltonian constraint and S^j as spatial reference fields for the diffeomorphism constraint. These observables depend on physical temporal and spatial coordinates τ and σ^j respectively and $\mathcal{O}_f(\tau,\sigma^j)$ has the interpretation that it returns the values of the phase space function f when the reference fields T, S^j take the values τ, σ^j underlying the relational formulation of the model.

[1] Note that we use different letters for these constraints during the treatment of the Gowdy model. This is done to be in line with the literature we want to compare our results to. Like introduced in Section 2.5, one typically uses $C_{\ldots}$ for the constraints in the framework of reduced phase space quantisation and the index 0 or no index for the Hamiltonian constraint specifically.

Because all Dirac observables $\mathcal{O}_f$ by construction commute with the canonical Hamiltonian, their dynamics in τ is generated by a so-called physical Hamiltonian H_{phys} via

$$\frac{\partial \mathcal{O}_f(\tau,\sigma)}{\partial \tau} = \{\mathcal{O}_f(\tau,\sigma), H_{\text{phys}}\}, \tag{4.3}$$

where for the Gaussian dust model the physical Hamiltonian reads

$$H_{\text{phys}} = \int_{\mathcal{S}} \mathrm{d}^3\sigma \, \mathcal{O}_C \tag{4.4}$$

and the integral is taken over the manifold coordinatised by the spatial dust reference fields, also called the dust space $\mathcal{S}$. This setup will be our starting point for the symmetry reduction in Section 4.2. In order to keep a more compact notation, we continue using $(\mathcal{A}, X, Y, \mathcal{E}, E^x, E^y)$, (C_θ, C) and (θ, x, y) instead of $(\mathcal{O}_{\mathcal{A}}, \mathcal{O}_X, \ldots, \mathcal{O}_{E^y})$, $(\mathcal{O}_{C_\theta}, \mathcal{O}_C)$ and $\big(\sigma^\theta, \sigma^x, \sigma^y\big)$ in the remaining part of this work.

4.2 Brief review of the symmetry reduction to a model with polarised $\mathbb{T}^3$ Gowdy symmetry

We start by introducing the basic elementary observables of the *Gowdy model* in loop quantum gravity along the seminal work of [152, 155, 197] carried over to the reduced phase space considered here, while we follow [163, 164, 198] the closest concerning notation.

Denoting the two Killing vector fields by $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$ and the remaining cyclic variable by θ, we decompose the connection and its conjugate momentum accordingly:

$$A = A^i_\theta(\theta)\tau_i \, \mathrm{d}\theta + A^i_\rho \tau_i \mathrm{d}x^\rho, \tag{4.5}$$

$$E = E^\theta_i(\theta)\tau_i \partial_\theta + E^\rho_i(\theta)\tau_i\partial_\rho. \tag{4.6}$$

Therein, we sum over x and y via ρ and $x^x := x, x^y := y$, while i takes the values 1, 2 and 3. Additionally, $\tau_i = -\frac{\mathrm{i}}{2}\sigma_i$ are the generators of $\mathfrak{su}(2)$, with the Pauli matrices σ_i.

The unpolarised Gowdy model, where the Killing vector fields are not demanded to be orthogonal, is then obtained via the choice

$$E^\theta_I = E^\rho_3 = 0 \text{ and}$$

$$A_\theta^I = A_\rho^3 = 0, \tag{4.7}$$

where the capital I is now representing 1 and 2. With this set of variables, the Gauß constraints G_1 and G_2 are trivially satisfied. The same holds for the geometric contributions to the spatial diffeomorphism constraints C_x and C_y. Within the relational formalism this is taken into account by the fact that we couple only two additional dust fields T, S^θ in the symmetry reduced sector, both depending on the θ coordinate only and thus there is no contribution from P_x, P_y in the total diffeomorphism constraints. The remaining geometric contributions to the total constraints involving gravity and dust at this stage read

$$G_3 = \frac{4\pi^2}{\kappa\beta_{\mathrm{BI}}}\big(\partial_\theta E_3^\theta + \epsilon_{3J}{}^K A_\rho^J E_K^\rho\big) =: \frac{1}{\kappa'\beta_{\mathrm{BI}}}\big(\partial_\theta E_3^\theta + \epsilon_{3J}{}^K A_\rho^J E_K^\rho\big), \tag{4.8}$$

$$C_\theta = \frac{1}{\kappa'\beta_{\mathrm{BI}}}\big(E_I^\rho\big(\partial_\theta A_\rho^I\big) + \epsilon_{3J}{}^K A_\rho^J E_K^\rho A_\theta^3 - \kappa\beta_{\mathrm{BI}} A_\theta^3 G_3\big), \tag{4.9}$$

$$\begin{aligned} C = &\frac{1}{2\kappa'\sqrt{\det E}}\big(2A_\theta^3 E_3^\theta A_\rho^J E_J^\rho + A_\rho^J E_J^\rho A_\sigma^K E_K^\sigma - A_\rho^K E_J^\rho A_\sigma^J E_K^\sigma - 2\epsilon_{3J}{}^K\big(\partial_\theta A_\rho^J\big) E_K^\rho E_3^\theta \\ &- \big(1+\beta_{\mathrm{BI}}^2\big)\big(2K_\theta^3 E_3^\theta K_\rho^J E_J^\rho + K_\rho^J E_J^\rho K_\sigma^K E_K^\sigma - K_\rho^K E_J^\rho K_\sigma^J K_\sigma^J E_K^\sigma\big)\big), \end{aligned} \tag{4.10}$$

where we have introduced $\det E := E_3^\theta(E_1^x E_2^y - E_2^x E_1^y)$ and $\kappa' := \frac{\kappa}{4\pi^2}$. The latter absorbs an additional factor of $4\pi^2$ that stems from smearing over the two variables x and y the model does not depend on anymore. In that sense, we solved already two of the integrals in (4.4).

We then proceed towards our final description via two canonical transformations. For the first one, we perform a polar decomposition of the A_ρ^I and E_I^ρ according to

$$\begin{aligned} &A_x^1 =: A_x\cos(\alpha+\beta), \quad A_y^1 =: -A_y\sin\big(\bar\alpha+\bar\beta\big), \quad E_1^x =: E^x\cos\beta, \quad E_1^y =: -E^y\sin\bar\beta, \\ &A_x^2 =: A_x\sin(\alpha+\beta), \quad A_y^2 =: A_y\cos\big(\bar\alpha+\bar\beta\big), \quad E_2^x =: E^x\sin\beta, \quad E_2^y =: E^y\cos\bar\beta, \end{aligned} \tag{4.11}$$

and as a result define

$$\begin{aligned} X &:= A_x\cos\alpha, & P^\beta &:= -E^x A_x\sin\alpha, \\ Y &:= A_y\cos\bar\alpha, & \bar P^\beta &:= -E^y A_y\sin\bar\alpha, \\ \mathcal{A} &:= \frac{1}{\beta_{\mathrm{BI}}}A_\theta^3, & \mathcal{E} &:= E_3^\theta. \end{aligned} \tag{4.12}$$

Then, the second canonical transformation reads

$$\begin{aligned} \xi &:= \beta - \bar{\beta}, & P^{\xi} &:= \frac{P^{\beta} - \bar{P}^{\beta}}{2}, \\ \eta &:= \beta + \bar{\beta}, & P^{\eta} &:= \frac{P^{\beta} + \bar{P}^{\beta}}{2}, \end{aligned} \tag{4.13}$$

resulting in the five pairs of canonically conjugate variables $(\mathcal{A}, \mathcal{E})$, (X, E^x), (Y, E^y), (η, P^η) and (ξ, P^ξ). Since the remaining diffeomorphism constraint C_θ^{tot} and the Hamiltonian constraint C^{tot} are reduced at the classical level by means of constructing Dirac observables, the only left first class constraint is the Gauss constraint G_3. The latter reduced two degrees of freedom in phase space such that for the unpolarised Gowdy model we end up with four physical degrees of freedom.

The polarised $\mathbb{T}^3$ Gowdy model can now be constructed by taking a look at the line element up to this point,

$$\mathrm{d}s^2 = \frac{E^x E^y}{E_3^\theta} \cos\xi \, \mathrm{d}\theta^2 + \frac{E_3^\theta E^y}{E^x \cos\xi} \mathrm{d}x^2 + \frac{E_3^\theta E^x}{E^y \cos\xi} \mathrm{d}y^2 - 2E_3^\theta \frac{\sin\xi}{\cos\xi} \mathrm{d}x \, \mathrm{d}y, \tag{4.14}$$

and demanding the $\mathrm{d}x\,\mathrm{d}y$-term to vanish. This can be realised by imposing the constraints

$$\xi(\theta) \approx 0 \quad \text{and} \tag{4.15}$$

$$\dot{\xi}(\theta) \approx 0, \tag{4.16}$$

where the latter guarantees the stability of the former. We get

$$\chi(\theta) := \dot{\xi}(\theta) = 2P^\xi + E_3^\theta \, \partial_\theta \ln \frac{E^y}{E^x}, \tag{4.17}$$

which fixes the conjugate momentum P^ξ and also results in $\dot{\chi}(\theta) \approx 0$ with no further ado. These polarisation constraints together with the Gauß constraint

$$G_3 = \frac{1}{\kappa' \beta_{\text{BI}}} (\partial_\theta \mathcal{E} + P^\eta) \tag{4.18}$$

complete the set of constraints. The symmetry reduced physical Hamiltonian then has the form

$$H_{\text{phys}} = \int_{\mathcal{S}^1} \mathrm{d}\theta \, C(\theta), \tag{4.19}$$

where $\mathcal{S}^1$ denotes the symmetry reduced dust space. The geometric contributions to the Hamilton constraint in terms of the Dirac observables now read

$$C = -\frac{1}{\kappa'\sqrt{\det E}}\left(\frac{1}{\beta_{\mathrm{BI}}^2}(XE^xYE^y + \mathcal{A}\mathcal{E}(XE^x+YE^y) + \mathcal{E}\partial_\theta\eta(XE^x+YE^y)) \right.$$
$$\left. + \frac{1}{4}\partial_\theta\mathcal{E} - \frac{1}{4}\left(\mathcal{E}\partial_\theta \ln\frac{E^y}{E^x}\right)^2\right) +$$
$$+ \frac{1}{\kappa'}\partial_\theta\left(\frac{\mathcal{E}\partial_\theta\mathcal{E}}{\sqrt{\det E}}\right) - \frac{\kappa'}{4}\frac{{G_3}^2}{\sqrt{\det E}} - \frac{\beta_{\mathrm{BI}}}{2}\partial_\theta\frac{G_3}{\sqrt{\det E}}, \tag{4.20}$$

where $\det E = \mathcal{E}E^xE^y$. Note that the other two integrations were already dealt with before, in (4.10). For completeness, we also present the geometric contribution to the diffeomorphism constraint in the symmetry reduced Gowdy model that takes the form

$$C_\theta = \frac{1}{\kappa'\beta_{\mathrm{BI}}}\left(E^\rho_I\left(\partial_\theta A^I_\rho\right) + \epsilon_{3J}{}^K A^J_\rho E^\rho_K A^3_\theta - \kappa\beta_{\mathrm{BI}}A^3_\theta G_3\right) \tag{4.21}$$

but does not contribute to the physical Hamiltonian in the case of the Gaussian dust model.

When it comes to the Gauß constraint, we may solve it already at this (classical) level. Noticing that η is just translated via the action of the Gauß constraint, we can impose $\eta \approx 0$. With the Gauß constraint G_3 and η being second class, we proceed with the Dirac bracket and make the two constraints vanish strongly. For all other quantities that do not depend on η, the Dirac bracket reduces to the Poisson bracket and nothing more has to be done.[2] Following this route, we end up with three independent pairs of elementary Dirac observables: $(\mathcal{A},\mathcal{E})$, (X, E^x) and (Y, E^y). Alternatively, as shown in [196, 197], the Gauß constraint can also easily be solved at the quantum level. In this case, operators associated with (η, P^η) will be involved in the kinematical Hilbert space and after solving the Gauß constraint the subspace of the kinematical Hilbert space no longer contains these quantum degrees of freedom.

[2]Note that $G_3 = 0$ allows to solve P^η for variables independent of η and P^η.

Chapter 5

Quantisation of the reduced LQG model with polarised $\mathbb{T}^3$ Gowdy symmetry

5.1 The physical Hilbert space in reduced LQG

As discussed in the former chapter, the physical phase space of the polarised Gowdy model involves three independent pairs of canonically conjugate Dirac observables after solving the Gauß constraint: $(\mathcal{A}, \mathcal{E})$, (X, E^x) and (Y, E^y). Imposing the polarisation condition eliminated (ξ, P^ξ) and, accordingly, fulfilling the Gauß constraint made (η, P^η) vanish. Since the algebra of these Dirac observables is given by the standard Poisson bracket we can use the same representations that was used in [164, 196] for the kinematical Hilbert space for the physical Hilbert space:

$$\mathcal{H}_{\text{phys}} = L_2(\overline{\mathcal{A}}_{\mathcal{S}^1 \times T^2}, \mu_0),$$

where $\overline{\mathcal{A}}_{\mathcal{S}^1 \times T^2}$ denotes the space of generalised connections on $T^3 \simeq \mathcal{S}^1 \times T^2$ and μ_0 is the analogue of the Ashtekar–Lewandowski measure in full LQG. $\overline{\mathcal{A}}_{\mathcal{S}^1 \times T^2}$ is constructed as follows: We consider $\mathcal{A}_{\mathcal{S}^1}$ and its projective limit over graphs Γ in $\mathcal{S}^1$, which are just non-intersecting unions of edges e_n that correspond to arcs here. A graph Γ is then given by $\Gamma = \cup_i e_i$. We denote by $V(\Gamma)$ the graph's set of vertices, which is just the union of all end points of the e_i, and by $E(\Gamma)$ its set of edges. For a given graph Γ we can understand the space $\mathcal{A}^{\Gamma}_{\mathcal{S}^1}$ as a set of maps from $E(\Gamma)$ to $U(1)^{|E(\Gamma)|}$, that is one copy of U(1) for each edge of the graph. For a fixed edge we have

$$\mathcal{A}_{\mathcal{S}^1} : \Gamma \to \mathrm{U}(1), e \mapsto h_e^{(k_e)}(\mathcal{A}) := \exp\left(\mathrm{i}\frac{k_e}{2}\int_e \mathcal{A}\right), \tag{5.1}$$

where the U(1) charges $k_e \in \mathbb{Z}$ and, for later convenience, a factor $\frac{1}{2}$ is introduced. Using that the set of graphs is a partially ordered directed set and introducing the projections $P_{\Gamma\Gamma'} : \mathcal{A}^{\Gamma}_{\mathcal{S}^1} \to \mathcal{A}^{\Gamma'}_{\mathcal{S}^1}, \mathcal{A} \mapsto P_{\Gamma\Gamma'}(\mathcal{A}^{\Gamma}) := \mathcal{A}^{\Gamma}\big|_{\Gamma'}$ for $\Gamma' \leq \Gamma$ one can derive the set of generalised connections $\overline{\mathcal{A}}_{\mathcal{S}^1}$ as the projective limit over graphs in $\mathcal{S}^1$, that is

$$\overline{\mathcal{A}}_{\mathcal{S}^1} = \lim_{\substack{\longleftarrow \\ \Gamma\subset\mathcal{S}^1}} \mathcal{A}^{\Gamma}_{\mathcal{S}^1}.$$

X and Y, in turn, are scalar fields and in order to still obtain a similar description, we follow [164, 197] and define so-called point holonomies [199]

$$h_v^{(\mu_v)}(X) := \exp\left(\mathrm{i}\frac{\mu_v}{2}X(v)\right) \quad \text{and} \tag{5.2}$$

$$h_v^{(\nu_v)}(Y) := \exp\left(\mathrm{i}\frac{\nu_v}{2}Y(v)\right) \tag{5.3}$$

sitting on the graph's vertices v with corresponding charges $\mu_v, \nu_v \in \mathbb{R}$ and with $X(v), Y(v) \in \mathbb{R}$. For each fixed vertex v, the space $C(\overline{\mathbb{R}}_{\mathrm{Bohr}})$ of continuous almost periodic functions on the Bohr compactification of the real line is used. The space of generalised connections $\overline{\mathcal{A}}_{T^2}$ can be obtained again as a projective limit, this time over the vertex set $V(\Gamma)$. For a fixed graph Γ, the space $\mathcal{A}^{\Gamma}_{T^2}$ involves maps from $V(\Gamma)$ to $(\overline{\mathbb{R}}_{\mathrm{Bohr}} \times \overline{\mathbb{R}}_{\mathrm{Bohr}})^{|V(\Gamma)|}$. For a fixed vertex v, we have $A_{T^2} : V(\Gamma) \to \overline{\mathbb{R}}_{\mathrm{Bohr}} \times \overline{\mathbb{R}}_{\mathrm{Bohr}}$ with $v \mapsto (X(v), Y(v))$. Then we have $\overline{\mathcal{A}}_{\mathcal{S}^1\times T^2} = \lim\limits_{\substack{\longleftarrow \\ \Gamma\subset\mathcal{S}^1}} \mathcal{A}^{\Gamma}_{\mathcal{S}^1} \otimes \mathcal{A}^{\Gamma}_{T^2}$.

The basis states of $\mathcal{H}_{\mathrm{phys}}$ are then labelled by a graph Γ — defining the sets of the vertices $V(\Gamma)$ and the edges $E(\Gamma)$ —, the U(1)-charges k_e (collected in k) as well as the point holonomies' charges μ_v and ν_v (collected in μ and ν respectively) [164]:

$$|\Gamma, k, \mu, \nu\rangle := \prod_{e\in E(\Gamma)} \exp\left(\mathrm{i}\frac{k_e}{2}\int_e \mathcal{A}\right) \prod_{v\in V(\Gamma)} \exp\left(\mathrm{i}\frac{\mu_v}{2}X(v)\right)\exp\left(\mathrm{i}\frac{\nu_v}{2}Y(v)\right). \tag{5.4}$$

We now use Figure 5.1 — showing exemplarily a five-valent Gowdy state in reduced LQG where we work with embedded graphs — to introduce the states' composition and notation. The dashed miniature lines in Figure 5.1 visualise the fact that the point holonomies are actually not along edges.

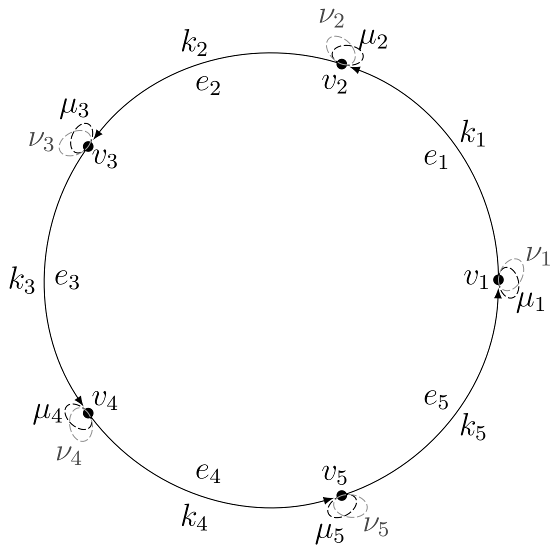


Figure 5.1: An embedded five-valent graph with charges k_e on the edges and point holonomies labelled by μ_v, ν_v on the vertices, serving as a basis element for Gowdy states. To keep the notation more compact, we used $k_{e_{v_I}} =: k_I, \mu_{v_I} =: \mu_I$ and $\nu_{v_I} =: \nu_I$.

The physical Hilbert space $\mathcal{H}_{\text{phys}}$ can also be written as a direct sum of the Hilbert spaces $\mathcal{H}_\Gamma$ associated to each graph $\Gamma \in \mathcal{S}^1$:

$$\mathcal{H}_{\text{phys}} = \bigoplus_{\Gamma} \mathcal{H}_\Gamma. \tag{5.5}$$

The holonomy operators act on the basis states (5.4) via multiplication:

$$\hat{h}^{(k_0)}_{e_I}(\mathcal{A})|\Gamma, k, \mu, \nu\rangle = \exp\left(\mathrm{i}\frac{k_0}{2}\int_{e_I} \mathcal{A}\right)|\Gamma, k, \mu, \nu\rangle = |\Gamma, k_{e_I} + k_0, \mu, \nu\rangle, \tag{5.6}$$

$$\hat{h}^{(\mu_0)}_{v_I}(X)|\Gamma, k, \mu, \nu\rangle = \exp\left(\mathrm{i}\frac{\mu_0}{2}X(v_I)\right)|\Gamma, k, \mu, \nu\rangle = |\Gamma, k, \mu_{v_I} + \mu_0, \nu\rangle, \tag{5.7}$$

$$\hat{h}^{(\nu_0)}_{v_I}(Y)|\Gamma, k, \mu, \nu\rangle = \exp\left(\mathrm{i}\frac{\nu_0}{2}Y(v_I)\right)|\Gamma, k, \mu, \nu\rangle = |\Gamma, k, \mu, \nu_{v_I} + \nu_0\rangle. \tag{5.8}$$

Therein, we used the abbreviation $k_{e_I} + k_0 =: k|_{k_{e_I} = k_{e_I} + k_0}$ within the state and likewise for μ and ν.

The according flux operators are implemented as follows. First, we have [164]

$$\hat{\mathcal{E}}(\theta)|\Gamma,k,\mu,\nu\rangle = -\mathrm{i}\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2\frac{\delta}{\delta\mathcal{A}(\theta)}|\Gamma,k,\mu,\nu\rangle = \frac{\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2}{2}\frac{k_{e^+(\theta)}+k_{e^-(\theta)}}{2}|\Gamma,k,\mu,\nu\rangle, \tag{5.9}$$

where $k_{e^+(\theta)}$ is the U(1)-charge of the edge that is outgoing at θ and $k_{e^-(\theta)}$ the one of the incoming edge. If θ does not coincide with a vertex, the two are the same and the factor $\frac{1}{2}$ vanishes.

For the x- and y-flux, we first of all smear them over intervals $\mathcal{I}$,

$$\hat{\mathcal{F}}_{x,\mathcal{I}} := \int_{\mathcal{I}} \hat{E}^x \quad \text{and} \tag{5.10}$$

$$\hat{\mathcal{F}}_{y,\mathcal{I}} := \int_{\mathcal{I}} \hat{E}^y, \tag{5.11}$$

to finally obtain [164]

$$\hat{\mathcal{F}}_{x,\mathcal{I}}|\Gamma,k,\mu,\nu\rangle = \frac{\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2}{2}\sum_{v\in V(\Gamma\cap\mathcal{I})}\mu_v|\Gamma,k,\mu,\nu\rangle \quad \text{and} \tag{5.12}$$

$$\hat{\mathcal{F}}_{y,\mathcal{I}}|\Gamma,k,\mu,\nu\rangle = \frac{\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2}{2}\sum_{v\in V(\Gamma\cap\mathcal{I})}\nu_v|\Gamma,k,\mu,\nu\rangle. \tag{5.13}$$

Therein, we collected all contributions of vertices that lie in the union of $\mathcal{I}$ and Γ. We get a factor $\frac{1}{2}$ if an endpoint of $\mathcal{I}$ coincides with a vertex. We will later, however, use intervals that contain one vertex at most, as this simplifies the transition towards the AQG framework presented in Chapter 6.

Before approaching the dynamics and the Hamiltonian constraint, we shortly illustrate how to deal with the Gauß constraint had it not been solved on the classical level already. Then, the pair (η, P^η) would still be part of the set of variables. Similar to the other variables, the point holonomy

$$h_v^{(\lambda_v)}(\eta) := \exp(\mathrm{i}\lambda_v\eta(v)) \ , \ \lambda_v \in \mathbb{Z} \ , \tag{5.14}$$

as well as the flux

$$\mathcal{F}_{\eta,\mathcal{I}} := \int_{\mathcal{I}} P^\eta \tag{5.15}$$

are defined. The corresponding holonomy operator $\hat{h}_v^{(\lambda_v)}(\eta)$ acts multiplicatively on the basis states, whose composition (5.4) is now additionally enriched with the holonomies $\exp(\mathrm{i}\lambda_v\eta(v))$ — denoted as $|\Gamma, k, \mu, \nu, \lambda\rangle$. Accordingly, the corresponding flux operator $\hat{\mathcal{F}}_{\eta,\mathcal{I}}$ acts via differentiation:

$$\hat{\mathcal{F}}_{\eta,\mathcal{I}}|\Gamma, k, \mu, \nu, \lambda\rangle = \beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2 \sum_{v\in V(\Gamma\cap\mathcal{I})} \lambda_v|\Gamma, k, \mu, \nu, \lambda\rangle. \tag{5.16}$$

We can then use these quantities to quantise the Gauß constraint (4.18) by means of choosing a suitable partition $\mathcal{P}(\epsilon)$ of $\mathcal{S}^1$ in terms of intervals $\mathcal{I}_n$ such that $\mathcal{S}^1 = \cup_n\mathcal{I}_n$ with $\mathcal{I}_n : [\theta_n - \frac{\epsilon}{2}, \theta_n + \frac{\epsilon}{2}]$. We can then obtain a regularisation of the Gauß constraint à la [164]

$$G_3^\epsilon = \frac{1}{\kappa'\beta_{\mathrm{BI}}} \sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)} \int_{\mathcal{I}_n} (\partial_\theta\mathcal{E} + P^\eta)\,\mathrm{d}\theta \tag{5.17}$$

$$= \frac{1}{\kappa'\beta_{\mathrm{BI}}} \sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)} \left(\mathcal{E}\left(\theta_n + \frac{\epsilon}{2}\right) - \mathcal{E}\left(\theta_n - \frac{\epsilon}{2}\right) + \mathcal{F}_{\eta,\mathcal{I}_n}\right) \tag{5.18}$$

$$\tag{5.19}$$

and in the limit when we send the regulator to zero we rediscover the classical Gauß constraint, that is

$$G_3 = \frac{1}{\kappa'\beta_{\mathrm{BI}}} \int_{\mathcal{S}^1} (\partial_\theta\mathcal{E} + P^\eta)\,\mathrm{d}\theta = \lim_{\epsilon\to 0} G_3^\epsilon. \tag{5.20}$$

The corresponding Gauß constraint operator is then obtained as

$$\widehat{G_3} := \lim_{\epsilon\to 0} \frac{1}{\kappa'\beta_{\mathrm{BI}}} \sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)} \left(\hat{\mathcal{E}}\left(\theta_n + \frac{\epsilon}{2}\right) - \hat{\mathcal{E}}\left(\theta_n - \frac{\epsilon}{2}\right) + \hat{\mathcal{F}}_{\eta,\mathcal{I}_n}\right). \tag{5.21}$$

Note that this Gauß operator agrees in its symmetric definition with the one used in [197], while it differs in this aspect to the one used in [164].

In the limit where we send the regulator to zero, also known as the infinite refinement limit, we can choose the partition fine enough such that at most one vertex is contained in $\mathcal{I}_n$. Then, the action of this Gauß constraint operator on the basis states reads [164]

$$\widehat{G_3}|\Gamma, k, \mu, \nu, \lambda\rangle = \frac{{\ell_{\mathrm{P}}}^2}{\kappa'} \sum_{v\in V(\Gamma)} \left(\frac{k_{e_v} - k_{e_{v^-}}}{2} + \lambda_v\right)|\Gamma, k, \mu, \nu, \lambda\rangle. \tag{5.22}$$

Therein and from now on, we use as convention for the notation of the k-labels that we always work with outgoing edges and therefore run through the vertices with respective superscripts. This means that the k-label of the ingoing edge at vertex v is the same as that of the outgoing edge at the left-neighbouring vertex v^-.

We can now solve the above Gauß constraint by imposing the following vertex-wise condition:

$$\lambda_v = -\frac{k_{e_v} - k_{e_{v^-}}}{2} , \quad \forall\, v \in V(\Gamma). \tag{5.23}$$

As $\lambda_v \in \mathbb{Z}$, the difference of the k-charges has to fulfil $k_{e_v} - k_{e_{v^-}} \in 2\mathbb{Z}$.

Note that from choosing an infinitely fine partition as above follows that if there is indeed a vertex within interval $\mathcal{I}_n$, there will be none in any of the two neighbouring intervals. Hence, in the action of the flux $\hat{\mathcal{E}}$ shown in (5.9), the two terms add up the same charge as it is just one edge that gets split up by $\theta_n - \frac{\epsilon}{2}$, or $\theta_n + \frac{\epsilon}{2}$ respectively, and not two different ones from one in- and one outgoing edge. This then leads to (5.22). We will later also show the implementation of a Gauß constraint operator in the AQG framework in Chapter 6, but nevertheless also there stick to the strategy of solving the Gauß constraint already on the classical level. This is foremost due to the fact that it can be solved straightforwardly, eliminating also one pair of canonically conjugate variables (η, P^η). So there really is no need to carry them along any further from this point onwards.

5.2 Quantum dynamics in the reduced LQG model

While the quantisation of $\mathrm{H}_{\mathrm{eucl}}$ and $\mathrm{H}_{\mathrm{lor}}$ is performed along the lines of [164], the transition to the AQG formalism for the Brown–Kuchar model and the master constraint respectively can be found in [200, 201]. Again, in terms of notation, we stay close to [163, 164] also used in [198]. As before, we first regularise the classical expression for the physical Hamiltonian H_{phys} in order to be able to define the corresponding operator on $\mathcal{H}_{\mathrm{phys}}$.

First of all and following [164, 196], we start with introducing the SU(2)-valued holonomies, which we can later use to reformulate $\mathrm{H}_{\mathrm{eucl}}$ and $\mathrm{H}_{\mathrm{lor}}$:

$$h_\theta(\mathcal{I}) \coloneqq \exp\left(\tau_3 k_0 \int_{\mathcal{I}} \mathcal{A}\right) = \cos\left(\frac{k_0}{2}\int_{\mathcal{I}} \mathcal{A}\right) + 2\tau_3 \sin\left(\frac{k_0}{2}\int_{\mathcal{I}} \mathcal{A}\right), \tag{5.24}$$

$$h_x(\theta) := \exp(\mu_0 \tau_x X) = \cos\Big(\frac{\mu_0}{2} X\Big) + 2\tau_x \sin\Big(\frac{\mu_0}{2} X\Big) \quad \text{and} \tag{5.25}$$

$$h_y(\theta) := \exp(\nu_0 \tau_y Y) = \cos\Big(\frac{\nu_0}{2} Y\Big) + 2\tau_y \sin\Big(\frac{\nu_0}{2} Y\Big). \tag{5.26}$$

Therein, we used

$$\begin{aligned} \tau_x(\theta) &:= \cos\beta(\theta)\tau_1 + \sin\beta(\theta)\tau_2 \quad \text{and} \\ \tau_y(\theta) &:= -\sin\beta(\theta)\tau_1 + \cos\beta(\theta)\tau_2, \end{aligned} \tag{5.27}$$

where the $\mathfrak{su}(2)$ basis $\tau_i = -\frac{\mathrm{i}}{2}\sigma_i$, $i = 1, 2, 3$, with the Pauli matrices σ_i satisfies

$$\begin{aligned} \operatorname{tr} \tau_i &= 0 \quad \text{and} \\ \tau_i \tau_j &= -\frac{1}{4}\delta_{ij} \mathbb{1}_{\mathrm{SU}(2)} + \frac{1}{2}\epsilon_{ijk}\tau_k. \end{aligned} \tag{5.28}$$

One can show the equality of the holonomies' splits into sine and cosine by using the easily verifiable identities

$$\tau_x{}^2 = \tau_y{}^2 = -\frac{1}{4}\mathbb{1}_{\mathrm{SU}(2)}. \tag{5.29}$$

Having the action of the basic operators at hand, we can proceed towards the quantisation of the physical Hamiltonian operator. But not before we address the volume operator, which will serve as a crucial ingredient of the Hamiltonian constraint operator. We follow again closely [164, 198]. As starting point, the volume of an arc $\mathcal{I}$ is classically given by the volume functional

$$V(\mathcal{I}) := 4\pi^2 \int_{\mathcal{I}} \mathrm{d}\theta \sqrt{|\det E|} = 4\pi^2 \int_{\mathcal{I}} \mathrm{d}\theta \sqrt{|\mathcal{E} E^x E^y|}. \tag{5.30}$$

Now, similar to the discussion of the Gauß constraint above, we choose a partition $\mathcal{P}(\epsilon)_{\mathcal{I}}$ of $\mathcal{I}$ into intervals $\mathcal{I}_n$ such that we have $\mathcal{I} = \cup_n \mathcal{I}_n$. This allows us to rewrite the volume functional as

$$V(\mathcal{I}) = 4\pi^2 \lim_{\epsilon\to 0} \sum_{\mathcal{I}_n \in \mathcal{P}(\epsilon)_{\mathcal{I}}} \int_{\mathcal{I}_n} \mathrm{d}\theta \sqrt{|\mathcal{E} E^x E^y|(\theta)} = 4\pi^2 \lim_{\epsilon\to 0} \sum_{\mathcal{I}_n \in \mathcal{P}(\epsilon)_{\mathcal{I}}} \int_{\theta_n - \frac{\epsilon}{2}}^{\theta_n + \frac{\epsilon}{2}} \mathrm{d}\tilde{\theta} \sqrt{|\mathcal{E} E^x E^y|(\tilde{\theta})}, \tag{5.31}$$

where we choose the intervals $\mathcal{I}_n$ sufficiently small, that is $\mathcal{I}_n = [\theta_n - \frac{\epsilon}{2}, \theta_n + \frac{\epsilon}{2}]$. The integral can then be replaced by a Riemann sum involving $\epsilon\sqrt{|\mathcal{E}E^xE^y|(\theta_n)}$, yielding for the regularised volume functional $V^\epsilon(\mathcal{I})$

$$\begin{aligned} V^\epsilon(\mathcal{I}) &= 4\pi^2 \sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)_\mathcal{I}} \sqrt{|\mathcal{E}||\epsilon E^x||\epsilon E^y|(\theta_n)} \\ &= 4\pi^2 \sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)_\mathcal{I}} \sqrt{|\mathcal{E}(\theta_n)|\left|\int_{\theta_n-\frac{\epsilon}{2}}^{\theta_n+\frac{\epsilon}{2}} E^x\right|\left|\int_{\theta_n-\frac{\epsilon}{2}}^{\theta_n+\frac{\epsilon}{2}} E^y\right|} \\ &= 4\pi^2 \sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)_\mathcal{I}} \sqrt{|\mathcal{E}(\theta_n)||\mathcal{F}_{x,\mathcal{I}_n}||\mathcal{F}_{y,\mathcal{I}_n}|}. \end{aligned} \tag{5.32}$$

From the first to the second line, we interpreted the two products including ϵ as approximations of infinitesimal integrals and then reintroduced the smeared fluxes $\mathcal{F}_{x,\mathcal{I}_n}, \mathcal{F}_{y,\mathcal{I}_n}$ — now with intervals labelled by n.

We then define the corresponding volume operator as

$$\hat{\mathrm{V}}(\mathcal{I}) = 4\pi^2 \lim_{\epsilon\to 0} \sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)_\mathcal{I}} \sqrt{\left|\hat{\mathcal{E}}(\theta_n)\right|\left|\hat{\mathcal{F}}_{x,\mathcal{I}_n}\right|\left|\hat{\mathcal{F}}_{y,\mathcal{I}_n}\right|}. \tag{5.33}$$

In the infinite refinement limit, we have at most one θ_n in each interval $\mathcal{I}_n$ and hence the action of $\hat{\mathrm{V}}(\mathcal{I})$ on the basic states states (5.4) in the physical Hilbert space is given by [164]

$$\hat{\mathrm{V}}(\mathcal{I})|\Gamma, k, \mu, \nu\rangle = \sum_{v\in V(\Gamma\cap\mathcal{I})} \hat{\mathrm{V}}_v\,|\Gamma, k, \mu, \nu\rangle, \tag{5.34}$$

where the sum involves all vertices of the graph Γ that lie in the interval $\mathcal{I}$ and we have

$$\hat{\mathrm{V}}_v\,|\Gamma, k, \mu, \nu\rangle = \frac{4\pi^2}{\sqrt{2}}\left(\frac{\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2}{2}\right)^{\frac{3}{2}} \sqrt{\left|k_{e_v} + k_{e_{v^-}}\right||\mu_v||\nu_v|}\,|\Gamma, k, \mu, \nu\rangle. \tag{5.35}$$

We can now turn to the regularisation and quantisation of the physical Hamiltonian H_{phys}. For this, we construct the Hamilton constraint by first integrating C over the dust manifold $\mathcal{S}$:

$$\mathrm{H}_{\mathrm{phys}} := \int_{\mathcal{S}^1} \mathrm{d}\theta C(\theta) = \int_{\mathcal{S}^1} \mathrm{d}\theta (C_{\mathrm{eucl}} + C_{\mathrm{lor}}) =: \mathrm{H}_{\mathrm{eucl}} + \mathrm{H}_{\mathrm{lor}}. \tag{5.36}$$

We thereby introduced the convenient split into a so-called Euclidean and Lorentzian part:

$$\begin{aligned}
C_{\text{eucl}} &:= C^{(1)}_{\text{eucl}} + C^{(2)}_{\text{eucl}} + C^{(3)}_{\text{eucl}} \\
C^{(1)}_{\text{eucl}} &:= -\frac{1}{\kappa' \beta^2_{\text{BI}}} \frac{1}{\sqrt{\det E}} (X E^x Y E^y) && (5.37) \\
C^{(2)}_{\text{eucl}} &:= -\frac{1}{\kappa' \beta^2_{\text{BI}}} \frac{1}{\sqrt{\det E}} (\mathcal{A}\mathcal{E} X E^x) && (5.38) \\
C^{(3)}_{\text{eucl}} &:= -\frac{1}{\kappa' \beta^2_{\text{BI}}} \frac{1}{\sqrt{\det E}} (\mathcal{A}\mathcal{E} Y E^y) && (5.39) \\
C_{\text{lor}} &:= C^{(1)}_{\text{lor}} + C^{(2)}_{\text{lor}} + C^{(3)}_{\text{lor}} \\
C^{(1)}_{\text{lor}} &:= -\frac{1}{4\kappa'} \frac{(\partial_\theta \mathcal{E})^2}{\sqrt{\det E}} && (5.40) \\
C^{(2)}_{\text{lor}} &:= \frac{1}{4\kappa'} \frac{\mathcal{E}^2}{\sqrt{\det E}} \left(\frac{\partial_\theta E^x}{E^x} - \frac{\partial_\theta E^y}{E^y} \right)^2 && (5.41) \\
C^{(3)}_{\text{lor}} &:= \frac{1}{\kappa'} \partial_\theta \left(\frac{\mathcal{E} \partial_\theta \mathcal{E}}{\sqrt{\det E}} \right). && (5.42)
\end{aligned}$$

We will now quantise H_{phys}, starting with the Euclidean part and continuing with the Lorentzian one. The final physical Hamiltonian operator will then be taken to be the symmetric combination that is $\hat{\text{H}}_{\text{phys}} = \frac{1}{2}\Big(\hat{\text{H}}_{\text{eucl}} + (\hat{\text{H}}_{\text{eucl}})^\dagger + \hat{\text{H}}_{\text{lor}} + (\hat{\text{H}}_{\text{lor}})^\dagger\Big)$ as can be seen in (5.78).

Note that the τ_x, τ_y can also be used to reformulate

$$E^x \tau_x = E^x_1 \tau_1 + E^x_2 \tau_2 \quad \text{and} \quad E^y \tau_y = E^y_1 \tau_1 + E^y_2 \tau_2 \tag{5.43}$$

of the x and y part of $E(\theta) = \mathcal{E}(\theta)\tau_3\partial_\theta + E^x(\theta)\tau_x(\theta)\partial_x + E^y(\theta)\tau_y(\theta)\partial_y$ and as they just result from a rotation of τ_2 and τ_3 in the 2-3-plane — which also explains (5.29) —, it furthermore still holds that

$$[\tau_x, \tau_y] = \tau_3, \quad [\tau_y, \tau_3] = \tau_x \quad \text{and} \quad [\tau_y, \tau_3] = -\tau_x. \tag{5.44}$$

A difference to the already existing quantisations of the Hamiltonian constraint in [164, 195] is that here we consider the physical Hamiltonian that at the classical level is invariant under spatial diffeomorphisms. If we aim at carrying over these symmetries also to the corresponding physical Hamiltonian operator, then, as pointed out in [58, 118] for the usual embedded LQG framework, we need to quantise H_{phys} in a graph-preserving way. Going back to the decomposition of the physical Hilbert space $\mathcal{H}_{\text{phys}}$ in terms of a direct sum of the individual graph Hilbert spaces $\mathcal{H}_\Gamma$ shown in (5.5), this means that the physical Hamiltonian operator $\hat{\text{H}}_{\text{phys}}$ will preserve each $\mathcal{H}_\Gamma$ separately, similar to the situation in full reduced LQG [61]. This can be achieved by using the notion of minimal loops originally introduced in [63, 64] that we will adapt to the symmetry reduced case of the polarised Gowdy model here. As discussed in [61], this has the consequence that the quantum theory involves infinitely many conserved charges that are absent in the classical theory and furthermore the physical Hilbert space is still non-separable in this model.

5.2.1 Quantisation of the Euclidean part of the physical Hamiltonian

We notice that $C_{\text{eucl}} = C^{(1)}_{\text{eucl}} + C^{(2)}_{\text{eucl}} + C^{(3)}_{\text{eucl}}$ consists of three similarly structured terms. Hence, we illustrate the regularisation procedure and the quantisation in detail for the first contribution $C^{(1)}_{\text{eucl}}$ of (5.37) only and then are more brief for the remaining two $C^{(2)}_{\text{eucl}}$ and $C^{(3)}_{\text{eucl}}$ since they can be obtained in a similar manner. As discussed in detail below, the regularisation chosen here is different from the one in [164] to ensure the graph-preserving property of the physical Hamiltonian operator $\hat{\text{H}}_{\text{phys}}$. Such a choice of regularisation is, however, closer to the way how H_{phys} will be quantised in the AQG framework discussed in Chapter 6.

We start with choosing a partition of S_1 and replacing the integral over $\mathcal{S}$ by a corresponding Riemann sum of intervals $\mathcal{I}_n = [\theta_n - \frac{\epsilon}{2}, \theta_n + \frac{\epsilon}{2}]$ with $\mathcal{S}^1 = \cup_n \mathcal{I}_n$ according to

$$\begin{aligned}
\text{H}^{(1)}_{\text{eucl}} &= \int_{\mathcal{S}^1} \mathrm{d}\theta\, C^{(1)}_{\text{eucl}} = -\frac{1}{\kappa' \beta^2_{\text{BI}}} \int_{\mathcal{S}^1} \mathrm{d}\theta \frac{X(\theta)E^x(\theta)Y(\theta)E^y(\theta)}{\sqrt{\det E(\theta)}} \\
&= -\frac{1}{\kappa' \beta^2_{\text{BI}}} \lim_{\epsilon\to 0} \sum_{\mathcal{I}_n \in \mathcal{P}(\epsilon)} \int_{\mathcal{I}_n} \mathrm{d}\theta \frac{X(\theta)E^x(\theta)Y(\theta)E^y(\theta)}{\sqrt{\det E(\theta)}} \\
&= -\frac{1}{\kappa' \beta^2_{\text{BI}}} \lim_{\epsilon\to 0} \sum_{\mathcal{I}_n \in \mathcal{P}(\epsilon)} \epsilon \frac{X(\theta_n)E^x(\theta_n)Y(\theta_n)E^y(\theta_n)}{\sqrt{\det E(\theta_n)}},
\end{aligned} \tag{5.45}$$

where we used in the last step that the intervals of the partition have length ϵ and can be chosen to be sufficiently small. Note that we could restrain ourselves to the integral of θ over $\mathcal{S}^1$ since all quantities only depend on θ. Also, we want to point out again our abuse of notation that is using $\sigma^\theta = \theta$ for the (cyclic) dust coordinate σ^θ on the dust manifold $\mathcal{S}^1$.

As the next step and following [164], we use that we can regularise the summand on the RHS of (5.45) à la

$$\begin{aligned}\frac{1}{4\pi^2}\,\mathrm{tr}\big(\big(h_x h_y {h_x}^{-1} {h_y}^{-1} - h_y h_x {h_y}^{-1} {h_x}^{-1}\big) h_\theta \big\{ {h_\theta}^{-1}, V(\mathcal{I}_n)\big\}\big) \\ = \frac{\kappa' \beta_{\mathrm{BI}}}{2} k_0 \mu_0 \nu_0 \epsilon \cdot \frac{XY E^x E^y}{\sqrt{\det E}}(\theta_n) + O(\epsilon^2, \mu_0^2, \nu_0^2),\end{aligned} \tag{5.46}$$

where $O(\epsilon^2, \mu_0^2, \nu_0^2)$ denotes all terms that involve at least second powers of either ϵ, μ_0 or ν_0 respectively. The expression in (5.46) transforms the term we started with into a straightforwardly quantisable expression of holonomies and the volume functional. This replacement neglects terms of second and higher orders in ϵ and holds for small $X, Y, \int_{\mathcal{I}} \mathcal{A}$ as we will see, where the smallness of the latter quantity corresponds to small intervals $\mathcal{I}$. Furthermore, tr denotes the SU(2) trace and the LHS depends of course on θ as well — we just refrain from writing down this dependency when the formulae become more elongate. Along the path after (5.30), restricting ourselves to infinitesimal intervals $\mathcal{I}_n$ around θ_n of length ϵ involved in the partition $\mathcal{P}(\epsilon)$ allows us to use the following form for the volume functional:

$$\begin{aligned}V(\mathcal{I}_n) &:= 4\pi^2 \int_{\mathcal{I}_n} \mathrm{d}\theta \sqrt{|\mathcal{E} E^x E^y|}(\theta) = 4\pi^2 \epsilon \sqrt{|\mathcal{E} E^x E^y|}(\theta_n) \\ &= 4\pi^2 \sqrt{|\mathcal{E}||\epsilon E^x||\epsilon E^y|}(\theta_n) = 4\pi^2 \sqrt{|\mathcal{E}| \left|\int_{\mathcal{I}_n} E^x\right| \left|\int_{\mathcal{I}_n} E^y\right|}.\end{aligned} \tag{5.47}$$

Then, we can compute the Poisson bracket of the θ-holonomy and the (infinitesimal) volume functional, which implies the Thiemann identity:

$$\begin{aligned}h_\theta \big\{ {h_\theta}^{-1}, V(\mathcal{I}_n)\big\} &= -\frac{\kappa' \beta_{\mathrm{BI}}}{2} k_0 \tau_3 \frac{\sqrt{\left|\int_{\mathcal{I}_n} E^x\right| \left|\int_{\mathcal{I}_n} E^x\right|}}{\sqrt{|\mathcal{E}|}} = -\frac{\kappa' \beta_{\mathrm{BI}}}{2} k_0 \tau_3 \frac{\left|\int_{\mathcal{I}_n} E^x\right| \left|\int_{\mathcal{I}_n} E^x\right|}{\frac{1}{4\pi^2} V(\mathcal{I}_n)} \\ &= -\frac{\kappa \beta_{\mathrm{BI}}}{2} k_0 \tau_3 \epsilon \frac{|E^x||E^x|}{\sqrt{\det E}}(\theta_n) + O(\epsilon^2).\end{aligned} \tag{5.48}$$

Note that we differ here from [164] by a factor of $4\pi^2$, while it is in line with [196].

The formula above already provides E^x and E^y for the RHS of (5.46). Next, we apply the approximation of small X, Y and $\int_{\mathcal{I}_n} \mathcal{A}$ to the sine and cosine formulation of the holonomies (5.24), (5.25) and (5.26):

$$h_\theta(\mathcal{I}_n) = 1 + \tau_3 k_0 \int_{\mathcal{I}_n} \mathcal{A} + O(\epsilon^2) = 1 + \tau_3 k_0 \epsilon \mathcal{A}(\theta_n) + O(\epsilon^2), \tag{5.49}$$

$$h_x(\theta_n) = 1 + \tau_x(\theta_n)\mu_0 X(\theta_n) + O(\mu_0^2) \;\text{ and} \tag{5.50}$$

$$h_y(\theta_n) = 1 + \tau_y(\theta_n)\nu_0 Y(\theta_n) + O(\nu_0^2). \tag{5.51}$$

With this, we get

$$h_x h_y {h_x}^{-1} {h_y}^{-1} - h_y h_x {h_y}^{-1} {h_x}^{-1} = 2\tau_3 \mu_0 \nu_0 X(\theta_n) Y(\theta_n) + O(\mu_0^2, \nu_0^2), \tag{5.52}$$

where $O(\mu_0^2, \nu_0^2)$ means terms that involve at least second powers of either μ_0 and/or ν_0 and taking the SU(2)-trace of this expression multiplied by (5.48) yields the result of (5.46). Note that it sufficed to expand the holonomies' trigonometric functions up to first order due to the multiplicative and subtractive structure of (5.52)'s LHS. Proceeding to the second order in the cosines only yields precisely these terms multiplied by the remaining holonomies' zeroth order terms as second order contribution. But these are then cancelled by the difference of the two products and hence there is no second order contribution other than the one above. Hence, the regularised expression for the first contribution denoted by $\mathrm{H}^{(1),\epsilon}_{\mathrm{eucl}}$ is given by

$$\mathrm{H}^{(1),\epsilon}_{\mathrm{eucl}} = -\frac{8\pi^2}{\kappa^2 \beta_{\mathrm{BI}}^3 k_0 \mu_0 \nu_0} \sum_{\mathcal{I}_n \in \mathcal{P}(\epsilon)} \mathrm{tr}\Big(\big(h_x h_y {h_x}^{-1} {h_y}^{-1} - h_y h_x {h_y}^{-1} {h_x}^{-1}\big) h_\theta \big\{ {h_\theta}^{-1}, V(\mathcal{I}_n)\big\}\Big). \tag{5.53}$$

The corresponding operator $\hat{\mathrm{H}}^{(1)}_{\mathrm{eucl}}$ is obtained in the limit where the regulator is removed and where we also take into account that we can define the operator separately for each graph Hilbert space $\mathcal{H}_\Gamma$, yielding

$$\hat{\mathrm{H}}^{(1)}_{\mathrm{eucl}} = \lim_{\epsilon\to 0} \hat{\mathrm{H}}^{(1),\epsilon}_{\mathrm{eucl}} = \lim_{\epsilon\to 0} \bigoplus_{\Gamma} \hat{\mathrm{H}}^{(1),\epsilon}_{\mathrm{eucl},\Gamma} = \bigoplus_{\Gamma} \hat{\mathrm{H}}^{(1)}_{\mathrm{eucl},\Gamma}, \tag{5.54}$$

with

$$\hat{\mathrm{H}}^{(1)}_{\mathrm{eucl},\Gamma} := \frac{8\pi^2 \mathrm{i}}{\ell_{\mathrm{P}}{}^2 \kappa k_0 \mu_0 \nu_0 \beta_{\mathrm{BI}}^3} \sum_{v \in V(\Gamma)} \mathrm{tr}\Big(\Big(\hat{h}_x \hat{h}_y \hat{h}_x{}^{-1} \hat{h}_y{}^{-1} - \hat{h}_y \hat{h}_x \hat{h}_y{}^{-1} \hat{h}_x{}^{-1} \Big) \hat{h}_\theta \Big[\hat{h}_\theta{}^{-1}, \hat{\mathrm{V}}_v \Big] \Big), \tag{5.55}$$

where the operator only acts on vertices due to the fact that the volume operator is involved — $\hat{\mathrm{V}}_v$ denotes the volume operator at vertex v as given in (5.35).

Continuing with the remaining two terms of $C^{(2)}_{\mathrm{eucl}}$ and $C^{(3)}_{\mathrm{eucl}}$ in (5.38) and (5.39) respectively, we first of all state the corresponding Thiemann identities

$$h_x \big\{ h_x{}^{-1}, V(\mathcal{I}_n) \big\} = -\frac{\kappa \beta_{\mathrm{BI}}}{2} \mu_0 \tau_x(\theta_n) \frac{\mathcal{E}|E^y|}{\sqrt{\det E}}(\theta_n) + O(\mu_0^2) \quad \text{and} \tag{5.56}$$

$$h_y \big\{ h_y{}^{-1}, V(\mathcal{I}_n) \big\} = -\frac{\kappa \beta_{\mathrm{BI}}}{2} \nu_0 \tau_y(\theta_n) \frac{\mathcal{E}|E^x|}{\sqrt{\det E}}(\theta_n) + O(\nu_0^2), \tag{5.57}$$

which again constitute one part of the terms' regularisation. In analogy to (5.52), we then find

$$h_\theta h_x h_\theta{}^{-1} h_x{}^{-1} - h_x h_\theta h_x{}^{-1} h_\theta{}^{-1} = 2 k_0 \mu_0 \epsilon \tau_y(\theta_n) \mathcal{A}(\theta_n) X(\theta_n) + O(\epsilon^2, \mu_0^2) \quad \text{and} \tag{5.58}$$

$$h_y h_\theta h_y{}^{-1} h_\theta{}^{-1} - h_\theta h_y h_\theta{}^{-1} h_y{}^{-1} = 2 k_0 \nu_0 \epsilon \tau_x(\theta_n) \mathcal{A}) \theta_n Y(\theta_n 0) + O(\epsilon^2, \nu_0^2). \tag{5.59}$$

Combining (5.56) with (5.59) and (5.57) with (5.58), we obtain

$$\begin{aligned} &\frac{1}{4\pi^2} \mathrm{tr}\Big(\big(h_y h_\theta h_y{}^{-1} h_\theta{}^{-1} - h_\theta h_y h_\theta{}^{-1} h_y{}^{-1} \big) h_x \big\{ h_x{}^{-1}, V(\mathcal{I}_n) \big\} \Big) \\ &\qquad = \frac{\kappa' \beta_{\mathrm{BI}}}{2} k_0 \mu_0 \nu_0 \epsilon \cdot \frac{\mathcal{A} Y \mathcal{E} E^y}{\sqrt{\det E}}(\theta_n) + O(\epsilon^2, \mu_0^2, \nu_0^2) \quad \text{and} \end{aligned} \tag{5.60}$$

$$\begin{aligned} &\frac{1}{4\pi^2} \mathrm{tr}\Big(\big(h_\theta h_x h_\theta{}^{-1} h_x{}^{-1} - h_x h_\theta h_x{}^{-1} h_\theta{}^{-1} \big) h_y \big\{ h_y{}^{-1}, V(\mathcal{I}_n) \big\} \Big) \\ &\qquad = \frac{\kappa' \beta_{\mathrm{BI}}}{2} k_0 \mu_0 \nu_0 \epsilon \cdot \frac{\mathcal{A} X \mathcal{E} E^x}{\sqrt{\det E}}(\theta_n) + O(\epsilon^2, \mu_0^2, \nu_0^2). \end{aligned} \tag{5.61}$$

However, to stick closer to [164, 198, 200, 201], we will use slightly different expressions. This is due to our choice of $\eta \approx 0$, which is not considered amongst the literature. Without fixing η, (5.38) and (5.39) are modified according to $\mathcal{A} \mapsto \mathcal{A} + \partial_\theta \eta$ and in order to be able to regularise the involved derivatives of η one has to work with shifted holonomies of the form $h_{x,\epsilon} = h_x(\theta_n + \epsilon)$.[1] However, the latter create new vertices in a given graph and thus cannot be used if we require the final physical Hamiltonian operator to be graph-preserving. As discussed above, in the Gaussian dust model this requirement is dictated by the classical symmetries of the physical Hamiltonian that we would like to implement also in the quantum model. Hence, if we aim at regularising in terms of shifted holonomies as well, then we need to consider a shift to the next vertex, that is $h_{x,\xi} = h_x(\theta_{n+\xi})$ where ξ can be chosen to be $\xi = \pm 1$ depending on whether the shift goes into the left or right direction from θ_n. That we only involve the next-neighbouring vertices corresponds to an analogue choice of a minimal loop that carries over to the choice of a minimal shift here. Now, in the former case where the shift involved the regularisation parameter ϵ, it was ensured that in the limit where we send the regulator to zero the size of the shift can be assumed to be very tiny. This is no longer given if we associated the shift with the two neighbouring points that will be identified with the corresponding vertices of a given graph in the quantum theory. Then only for those graphs where the edge length between two neighbouring vertices can be assumed to be tiny will the regularised expression yield a good approximation of the corresponding classical expression. Note that this causes no severe issue here because we will follow the same strategy as used in the AQG framework [58], although in a slightly different context. For the quantisation of the Euclidean part of the physical Hamiltonian part we do not require that the regularised expression reproduces the classical expression directly when we send the regulator to zero. Instead, we call an operator suitably quantised if for a chosen set of semiclassical states the corresponding expectation values reproduce in lowest order the correct classical expression. To judge this in detail, one needs to perform a semiclassical analysis of the relevant operators. However, even if we do not perform a detailed semiclassical computation here, using the existing results in [133–135] as well as [2, 3] we can already draw some conclusions here if we restrict our discussions to the lowest order only. A suitable choice of coherent states that we can consider here for each classical canonical pair are U(1) complexifier coherent states that were introduced in [133]. Their expectation values as well as their peakedness property have been analysed in [134, 135]. From these results we know that in the lowest order of the semiclassical parameter, corresponding to the classical limit where $\hbar$ is sent to zero, the expectation value of the holonomy operator agrees with the classical holonomy and the same holds also for point holonomies. Furthermore, using the results of [2, 3],

[1] Note that the formulae involving shifted holonomies are furthermore geometrically motivated. They approximate the corresponding curvature within the loops described by the holonomies. Hence the evaluation on θ or $\theta + \epsilon$ — depending on whether one travelled in θ-direction before or not.

we also know that the expectation values of the operator $\hat{h}[\hat{h}^{-1},\hat{V}]$ agrees in the lowest non-vanishing order of the semiclassical parameter with its classical counterpart. This motivates to define for the two remaining parts of the Euclidean physical Hamiltonian the following operators:

$$\hat{\mathrm{H}}^{(2)}_{\mathrm{eucl}} = \bigoplus_{\Gamma} \hat{\mathrm{H}}^{(2)}_{\mathrm{eucl},\Gamma} \quad \text{and} \quad \hat{\mathrm{H}}^{(3)}_{\mathrm{eucl}} = \bigoplus_{\Gamma} \hat{\mathrm{H}}^{(3)}_{\mathrm{eucl},\Gamma}, \tag{5.62}$$

with

$$\hat{\mathrm{H}}^{(2)}_{\mathrm{eucl},\Gamma} = \frac{8\pi^2 \mathrm{i}}{\ell_{\mathrm{P}}{}^2 \kappa k_0 \mu_0 \nu_0 \beta^3_{\mathrm{BI}}} \frac{1}{2} \sum_{\substack{v\in V(\Gamma)\\ \xi=\pm 1}} \mathrm{tr}\Big(\Big(\hat{h}_y \hat{h}_\theta \hat{h}_{y,\xi}{}^{-1} \hat{h}_\theta{}^{-1} - \hat{h}_\theta \hat{h}_{y,\xi} \hat{h}_\theta{}^{-1} \hat{h}_y{}^{-1}\Big) \hat{h}_x \Big[\hat{h}_x{}^{-1}, \hat{\mathrm{V}}_v\Big]\Big) \tag{5.63}$$

and

$$\hat{\mathrm{H}}^{(3)}_{\mathrm{eucl},\Gamma} = \frac{8\pi^2 \mathrm{i}}{\ell_{\mathrm{P}}{}^2 \kappa k_0 \mu_0 \nu_0 \beta^3_{\mathrm{BI}}} \frac{1}{2} \sum_{\substack{v\in V(\Gamma)\\ \xi=\pm 1}} \mathrm{tr}\Big(\Big(\hat{h}_\theta \hat{h}_{x,\xi} \hat{h}_\theta{}^{-1} \hat{h}_x{}^{-1} - \hat{h}_x \hat{h}_\theta \hat{h}_{x,\xi}{}^{-1} \hat{h}_\theta{}^{-1}\Big) \hat{h}_y \Big[\hat{h}_y{}^{-1}, \hat{\mathrm{V}}_v\Big]\Big), \tag{5.64}$$

where again the sum runs over all vertices v, we used $\kappa'\hbar = \ell_{\mathrm{P}}{}^2$ and we included an additional factor of $\frac{1}{2}$ because we considered $\xi = \pm 1$. Further, $\hat{h}_{x,\xi} = \hat{h}_x(v_\xi)$ and $\hat{h}_{y,\xi} = \hat{h}_y(v_\xi)$ where v_+ and v_- denote the neighbouring vertices of v to the right and left, respectively. Taking into account that these coherent states satisfy a resolution of identity together with their peakedness property [134, 135] as well as the results of semiclassical expectation values for U(1) coherent states of square root operators in terms of Kummer functions [2, 3], we can conclude that in the lowest order of the semiclassical parameter the operators $\hat{\mathrm{H}}^{(2)}_{\mathrm{eucl}}$ and $\hat{\mathrm{H}}^{(3)}_{\mathrm{eucl}}$ will reproduce the correct classical limit, that is

$$\begin{aligned}
&\langle \Psi^t_{(\mathcal{A},\mathcal{E},X,E^x,Y,E^y)} \,|\, \hat{\mathrm{H}}^{(I=2,3)}_{\mathrm{eucl}} \,|\, \Psi^t_{(\mathcal{A},\mathcal{E},X,E^x,Y,E^y)} \rangle = \\
&= 4\pi^2 \int_{\mathcal{S}^1} \mathrm{d}\theta\, C^{(I)}_{\mathrm{eucl}}(\mathcal{A}(\theta), \mathcal{E}(\theta), X(\theta), E^x(\theta), Y(\theta), E^y(\theta)) + O(t, \epsilon, \mu_0, \nu_0),
\end{aligned}$$

where one needs to choose a suitable set of coherent states such that the associated embedded graphs Γ in $\mathcal{S}^1$ involved in the definition of $\Psi^t_{(\mathcal{A},\mathcal{E},X,E^x,Y,E^y)}$ approximate $\mathcal{S}^1$ well enough when the sum over all vertices of the graphs is considered. We would like to emphasise that we can use former results on semiclassical computations here only because we quantised the physical Hamiltonian in a graph-preserving manner — suitable semiclassical states for graph-modifying operators in LQG are still an open and difficult question. Note that because we do not perform a detailed semiclassical computation here, we cannot make any statement about the terms involved in higher orders than the lowest order one. These can only be determined by computing the semiclassical expectation value in detail which, however, will not be part of this work. As discussed above, working with shifted holonomies is motivated by the fact that one needs to regularise the derivative of η being involved when the Gauß constraint is not solved at the classical level already. Since these formulae are still correct for $\eta \approx 0$, we will use these from now on, too, and thus enabling an easier transition between the two approaches. Note that for $\eta \approx 0$ we have $\tau_x(\theta) = \tau_1$ and $\tau_y(\theta) = \tau_2$ because the θ-dependent coefficients in (5.27) are either zero or one. Furthermore, this choice ensures that the operator obtained from following a Dirac quantisation procedure for the Gauß constraint and the one from the reduced quantisation considered here have the same regularisation. Because in the reduced case we could also choose a regularisation where the holonomy is located at the same vertices for all involved holonomies, we realise that such a choice is another example where Dirac and reduced quantisation would not yield the same final form of the operator similar to the situation discussed in [202], although the latter shows a stronger difference between the two cases.

Altogether, this results in

$$\begin{aligned}\hat{\mathrm{H}}_{\mathrm{eucl},\Gamma} = \frac{8\pi^2 \mathrm{i}}{\ell_{\mathrm{P}}{}^2 \kappa k_0 \mu_0 \nu_0 \beta_{\mathrm{BI}}^3} \sum_{v \in V(\Gamma)} \mathcal{P}_\Gamma \operatorname{tr}\Big(&\Big(\hat{h}_x \hat{h}_y \hat{h}_x{}^{-1} \hat{h}_y{}^{-1} - \hat{h}_y \hat{h}_x \hat{h}_y{}^{-1} \hat{h}_x{}^{-1}\Big) \hat{h}_\theta \Big[\hat{h}_\theta{}^{-1}, \hat{\mathrm{V}}_v\Big] \\ &+ \frac{1}{2} \sum_{\xi=\pm 1} \Big(\hat{h}_y \hat{h}_\theta \hat{h}_{y,\xi}{}^{-1} \hat{h}_\theta{}^{-1} - \hat{h}_\theta \hat{h}_{y,\xi} \hat{h}_\theta{}^{-1} \hat{h}_y{}^{-1}\Big) \hat{h}_x \Big[\hat{h}_x{}^{-1}, \hat{\mathrm{V}}_v\Big] \\ &+ \frac{1}{2} \sum_{\xi=\pm 1} \Big(\hat{h}_\theta \hat{h}_{x,\xi} \hat{h}_\theta{}^{-1} \hat{h}_x{}^{-1} - \hat{h}_x \hat{h}_\theta \hat{h}_{x,\xi}{}^{-1} \hat{h}_\theta{}^{-1}\Big) \hat{h}_y \Big[\hat{h}_y{}^{-1}, \hat{\mathrm{V}}_v\Big]\Big) \mathcal{P}_\Gamma,\end{aligned} \tag{5.65}$$

where we introduced in addition $\mathcal{P}_\Gamma : \mathcal{H}_{\mathrm{phys}} \to \mathcal{H}_\Gamma$, which are orthogonal projections that ensure that the operator is indeed graph-preserving if for instance two holonomies along a given edge combine to the identity. As before, $\hat{\mathrm{V}}_v$ denotes the volume operator at vertex v, (5.35). This finishes our discussion on the graph-preserving quantisation of the Euclidean part of the physical Hamiltonian.

5.2.2 Quantisation of the Lorentzian part of the physical Hamiltonian

Turning our attention to the quantisation of $\mathrm{H}_{\mathrm{lor}}$, we start again with the first part. According to (5.40) and choosing again a partition of $\mathcal{S}^1$ such that $\mathcal{S}^1 = \cup_n \mathcal{I}_n$ with $\mathcal{I}_n : [\theta_n - \frac{\epsilon}{2}, \theta_n + \frac{\epsilon}{2}]$, we have

$$\begin{aligned}
\mathrm{H}_{\mathrm{lor}}^{(1)} &= -\frac{1}{4\kappa'} \int_{\mathcal{S}^1} \mathrm{d}\theta \frac{(\partial_\theta \mathcal{E})^2}{\sqrt{\det E}}(\theta) \\
&= -\frac{1}{4\kappa'} \lim_{\epsilon\to 0} \sum_{\mathcal{I}_n \in \mathcal{P}(\epsilon)} \int_{\mathcal{I}_n} \mathrm{d}\theta \frac{(\partial_\theta \mathcal{E})^2}{\sqrt{\det E}}(\theta) \\
&= -\frac{1}{4\kappa'} \lim_{\epsilon\to 0} \sum_{\mathcal{I}_n \in \mathcal{P}(\epsilon)} \frac{(\epsilon \partial_\theta \mathcal{E}(\theta_n))^2}{\epsilon \sqrt{\det E(\theta_n)}} \\
&= -\frac{1}{4\kappa'} \lim_{\epsilon\to 0} \sum_{\mathcal{I}_n \in \mathcal{P}(\epsilon)} \frac{(\mathcal{E}(\theta_n + \epsilon) - \mathcal{E}(\theta_n))^2}{\frac{1}{4\pi^2} V(\mathcal{I}_n)}.
\end{aligned} \tag{5.66}$$

The last step then also used (5.47) for the volume of a tiny interval $\mathcal{I}_n$ around θ_n and $\mathcal{E}(\theta_n + \epsilon) = \mathcal{E}(\theta_n) + \epsilon \partial_\theta \mathcal{E}(\theta_n) + O(\epsilon^2)$ for the derivative expression.

The remaining task consists in dealing with the inverse volume involved in (5.66). For this purpose, we consider the Thiemann identity in (5.48) as well as the two analogue expressions in (5.56) and (5.57) and use the quantity $Z(\mathcal{I})$ introduced already in [164] to obtain

$$\begin{aligned}
Z(\mathcal{I}_n) &:= \epsilon^{abc} \operatorname{tr}\big(h_a \big\{ {h_a}^{-1}, V(\mathcal{I}_n) \big\} h_b \big\{ {h_b}^{-1}, V(\mathcal{I}_n) \big\} h_c \big\{ {h_c}^{-1}, V(\mathcal{I}_n) \big\}\big) \\
&= \frac{3}{2} \left(\frac{\kappa \beta_{\mathrm{BI}}}{2} \right)^3 k_0 \mu_0 \nu_0 V(\mathcal{I}_n) + O(\mu_0^2, \nu_0^2, \epsilon^2).
\end{aligned} \tag{5.67}$$

Following [164], we can then derive

$$\begin{aligned}
Z_r(\mathcal{I}_n) &:= \epsilon^{abc} \operatorname{tr}\big(h_a \big\{ {h_a}^{-1}, V^r(\mathcal{I}_n) \big\} h_b \big\{ {h_b}^{-1}, V^r(\mathcal{I}_n) \big\} h_c \big\{ {h_c}^{-1}, V^r(\mathcal{I}) \big\}\big) \\
&= \frac{3}{2} \left(\frac{\kappa \beta_{\mathrm{BI}}}{2} \right)^3 r^3 k_0 \mu_0 \nu_0 V^{3r-2}(\mathcal{I}_n) + O(\mu_0^2, \nu_0^2, \epsilon^2) \\
&= r^3 V^{3r-3}(\mathcal{I}_n) Z(\mathcal{I}_n) + O(\mu_0^2, \nu_0^2, \epsilon^2),
\end{aligned} \tag{5.68}$$

which allows us to introduce the following decomposition of unity:

$$(1)^l = \left(\frac{16}{3(\kappa\beta_{\mathrm{BI}})^3 k_0\mu_0\nu_0}\frac{Z(\mathcal{I}_n)}{V(\mathcal{I}_n)}\right)^l = \left(\frac{16}{3(\kappa\beta_{\mathrm{BI}})^3 k_0\mu_0\nu_0}\right)^l\left(\frac{Z_r(\mathcal{I})}{r^3 V^{3r-2}(\mathcal{I}_n)}\right)^l, \tag{5.69}$$

with $l \in \mathbb{R}$. We can now use this identity to eliminate the inverse volume in (5.66). Setting

$$(3r-2)l = -1 \quad \Rightarrow \quad r = \frac{2}{3} - \frac{1}{3l} \tag{5.70}$$

results in an inverse volume on the LHS of (5.69), which we then insert into (5.66) to obtain a regularised expression $\mathrm{H}^{(1),\epsilon}_{\mathrm{lor}}$ of the form:

$$\mathrm{H}^{(1),\epsilon}_{\mathrm{lor}} := -\frac{4\pi^2}{4\kappa'}\left(\frac{16}{3(\kappa\beta_{\mathrm{BI}})^3 r^3 k_0\mu_0\nu_0}\right)^l \sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)} \left(\mathcal{E}(\theta_n+\epsilon)-\mathcal{E}(\theta_n)\right)^2 {Z_r}^l(\mathcal{I}_n)\Big|_{r=\frac{2}{3}-\frac{1}{3l}}. \tag{5.71}$$

As for the Euclidean part, the corresponding operator $\hat{\mathrm{H}}^{(1)}_{\mathrm{lor}}$ is obtained in the limit where the regulator is removed. We take again the infinite refinement limit where at most on vertex is in each $\mathcal{I}_n$ and where we also take into account that we can define the operator separately for each graph Hilbert space $\mathcal{H}_\Gamma$, yielding

$$\hat{\mathrm{H}}^{(1)}_{\mathrm{lor}} = \lim_{\epsilon\to 0}\hat{\mathrm{H}}^{(1),\epsilon}_{\mathrm{lor}} = \lim_{\epsilon\to 0}\bigoplus_{\Gamma}\hat{\mathrm{H}}^{(1),\epsilon}_{\mathrm{lor},\Gamma} = \bigoplus_{\Gamma}\hat{\mathrm{H}}^{(1)}_{\mathrm{lor},\Gamma} \tag{5.72}$$

with

$$\begin{aligned}\hat{\mathrm{H}}^{(1)}_{\mathrm{lor},\Gamma}|\Gamma,k,\mu,\nu\rangle =& -\frac{4\pi^2}{4\kappa'}\left(\frac{-\mathrm{i}}{\hbar}\right)^{3l}\left(\frac{16}{3(\kappa\beta_{\mathrm{BI}})^3 r^3 k_0\mu_0\nu_0}\right)^l\cdot \\ &\cdot\sum_{v\in V(\Gamma)}\left(\left(k_{e_{v^+}}-k_{e_{v^-}}\right)\right)^2 {\hat{\mathrm{Z}}_{r,v}}{}^l\Big|_{r=\frac{2}{3}-\frac{1}{3l}}|\Gamma,k,\mu,\nu\rangle,\end{aligned} \tag{5.73}$$

where $k_{e_{v^+}}$ is the label attached to the outgoing edge of the vertex v^+ and $k_{e_{v^-}}$ is the label attached to the edge incoming at the vertex v — i.e. outgoing from vertex v^-. Furthermore, we used that the operator $\hat{\mathrm{Z}}_{r,v}$ [164] given by

$$\hat{\mathrm{Z}}_{r,v} := \epsilon^{abc}\,\mathrm{tr}\Big(\hat{h}_a\Big[\hat{h}_a{}^{-1},\hat{\mathrm{V}}^r_v\Big]\hat{h}_b\Big[\hat{h}_b{}^{-1},\hat{\mathrm{V}}^r_v\Big]\hat{h}_c\Big[\hat{h}_c{}^{-1},\hat{\mathrm{V}}^r_v\Big]\Big) \tag{5.74}$$

does not change the labels of the state $|\Gamma,k,\mu,\nu\rangle$ that it acts on.

In similar ways, we obtain the respective expressions for the second and third Lorentzian part:

$$\hat{\mathrm{H}}^{(2)}_{\mathrm{lor},\Gamma}|\Gamma,k,\mu,\nu\rangle = \frac{4\pi^2}{4\kappa'}\left(\frac{-\mathrm{i}}{\hbar}\right)^{3l}\left(\frac{16}{3(\kappa\beta_{\mathrm{BI}})^3 {r_2}^3 k_0\mu_0\nu_0}\right)^{l} \sum_{v\in V(\Gamma)}\left(k_{e_v}+k_{e_{v^-}}\right)^4\left(\mu_v\nu_{v_+}-\nu_v\mu_{v_+}\right)^2 \hat{\mathrm{Z}}_{r_2,v}{}^{l}\Big|_{r_2=\frac{2}{3}-\frac{5}{3l}}|\Gamma,k,\mu,\nu\rangle \tag{5.75}$$

$$\begin{aligned}\hat{\mathrm{H}}^{(3)}_{\mathrm{lor},\Gamma}|\Gamma,k,\mu,\nu\rangle = &\frac{4\pi^2}{\kappa'}\left(\frac{-\mathrm{i}}{\hbar}\right)^{3l}\left(\frac{16}{3(\kappa\beta_{\mathrm{BI}})^3 r^3 k_0\mu_0\nu_0}\right)^{l} \\ &\sum_{v\in V(\Gamma)}\Bigg(\left(k_{e_{v^+}}+k_{e_v}\right)\left(k_{e_{v^{++}}}-k_{e_v}\right)\hat{\mathrm{Z}}_{r,v_+}{}^{l}\Big|_{r=\frac{2}{3}-\frac{1}{3l}} - \\ &-\left(k_{e_v}+k_{e_{v^-}}\right)\left(k_{e_{v^+}}-k_{e_{v^-}}\right)\hat{\mathrm{Z}}_{r,v}{}^{l}\Big|_{r=\frac{2}{3}-\frac{1}{3l}}\Bigg)|\Gamma,k,\mu,\nu\rangle\end{aligned} \tag{5.76}$$

where v^{++} denotes the subsequent vertex after v^+. Note that we evaluate $\hat{\mathrm{Z}}$ within the second contribution $\hat{\mathrm{H}}^{(2)}_{\mathrm{lor},\Gamma}$ on a different value of $r_2 = \frac{2}{3} - \frac{5}{3l}$.

With that, the Lorentzian contribution to $\hat{\mathrm{H}}_{\mathrm{phys}}$ reads

$$\hat{\mathrm{H}}_{\mathrm{lor}} = \bigoplus_{\Gamma}\hat{\mathrm{H}}_{\mathrm{lor},\Gamma} = \bigoplus_{\Gamma}\hat{\mathrm{H}}^{(1)}_{\mathrm{lor},\Gamma}+\hat{\mathrm{H}}^{(2)}_{\mathrm{lor},\Gamma}+\hat{\mathrm{H}}^{(3)}_{\mathrm{lor},\Gamma} \tag{5.77}$$

and the physical Hamiltonian in the reduced loop quantum gravity Gowdy model finally takes the following form:

$$\hat{\mathrm{H}}_{\mathrm{phys}} = \bigoplus_{\Gamma}\hat{\mathrm{H}}_{\mathrm{phys},\Gamma} = \frac{1}{2}\bigoplus_{\Gamma}\left(\hat{\mathrm{H}}_{\mathrm{eucl},\Gamma} + (\hat{\mathrm{H}}_{\mathrm{eucl},\Gamma})^\dagger + \hat{\mathrm{H}}_{\mathrm{lor},\Gamma} + (\hat{\mathrm{H}}_{\mathrm{lor},\Gamma})^\dagger\right). \tag{5.78}$$

This finishes the discussion on the quantisation of the physical Hamiltonian of the Gowdy model in the reduced LQG framework.

Chapter 6

Quantisation of the model with polarised $\mathbb{T}^3$ Gowdy symmetry within Algebraic Quantum Gravity

As discussed in the previous Chapter 5, we needed to quantise the physical Hamiltonian in a graph-preserving way in order to carry over its classical symmetries to the quantum theory. In the case of reduced LQG, this corresponds to a quantisation that preserves each graph Hilbert space $\mathcal{H}_\gamma$ separately, yielding infinitely many conserved charges in the quantum theory that are absent in the classical theory. An alternative framework for the quantisation of these kind of operators where the graph-preserving feature of operators are implemented in a slightly different context is the algebraic quantum gravity (AQG) approach introduced in [58] and combined with a reduced phase space quantisation for full LQG in [61].

6.1 The physical Hilbert space in AQG

Here, we want to follow this quantisation approach in the symmetry reduced case of Gowdy models. One of the main difference is that AQG considers only one abstract infinite graph α, whereas we had to include infinitely many finite embedded graphs Γ for reduced LQG. The underlying Hilbert space in AQG is von-Neumann's infinite tensor product Hilbert space denoted by $\mathcal{H}_{\mathrm{ITP}}$ so that the physical Hilbert space in the AQG framework is

$\mathcal{H}_{\text{phys}} = \mathcal{H}_{\text{ITP}}$. The topology of the abstract graph is chosen to define the corresponding AQG model and here this means that for the analogue of a Gowdy state's LQG-graph like the one of Figure 5.1, we need to rearrange it to a line with the same number of charged vertices v_I, see Figure 6.1. To the right of every vertex v, the outgoing edge e_v is attached and hence, the respective incoming edge at vertex v is e_{v^-}. The charges k_{e_v}, μ_v and ν_v are then assigned correspondingly, with the only non-straightforward assignment being the one of edge e_{v_0}, incoming at v_1, which we have to charge with $k_{e_{v_N}}$, the charge at the edge e_{v_N}, in order to preserve the cyclic structure (cf. Fig. 5.1). All other edges and vertices are trivially charged and therefore do not contribute when operators such as the fluxes act on them. Note that Figure 6.1 shows again dashed miniature loops at the charged vertices representing the point holonomies in order to emphasise that they are not in fact holonomies along edges.

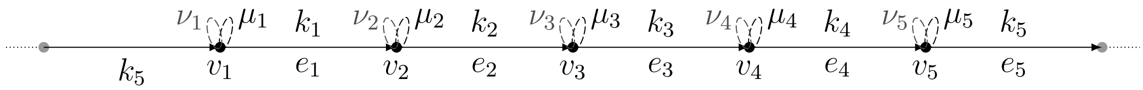


Figure 6.1: An abstract infinite AQG-graph, corresponding to the embedded one of Figure 5.1, with five vertices on which two point holonomies sit and six charged edges, where the most leftward one — the copy of k_5 — ensures the state's periodicity. Here, to keep the notation more compact, we used $k_{e_{v_I}} =: k_I, \mu_{v_I} =: \mu_I$ and $\nu_{v_I} =: \nu_I$.

In general, dynamical operators can be carried over from the embedded LQG framework to AQG if they are spatially diffeomorphism invariant. In the case of the Gowdy model, this corresponds to operators that involve integrals over the dust manifold $\mathcal{S}^1$. All operators — including the physical Hamiltonian — will be implemented graph-preserving by construction, but one of the differences to the reduced LQG case is that in AQG we allow trivial representations on the edges of the infinite abstract graph α.

Following the approach in [58], the holonomies, states and fluxes are introduced as follows. To each edge of the abstract infinite graph α we associate an U(1) element similar to the holonomy in (5.1) for reduced LQG, but with the difference that here we do not express the U(1) element in terms of an integral along the edges but we associate to a given edge e of the abstract graph α the U(1) element

$$h_e^{(k_e)}(\mathcal{A}) := \exp\left(\mathrm{i}\frac{k_e}{2}\mathcal{A}_e\right), \quad \text{with } \mathcal{A}_e \in \mathbb{R}. \tag{6.1}$$

Given this, we can define the analogue of the basis state in LQG shown in (5.4) now in the AQG framework as

$$|\alpha, k, \mu, \nu\rangle := \prod_{e\in E(\alpha)} \exp\Big(\mathrm{i}\frac{k_e}{2}\mathcal{A}_e\Big) \prod_{v\in V(\alpha)} \exp\Big(\mathrm{i}\frac{\mu_v}{2}X_v\Big)\exp\Big(\mathrm{i}\frac{\nu_v}{2}Y_v\Big), \tag{6.2}$$

where for the point holonomies we introduced the notation $X_v := X(v), Y_v := Y(v)$. The holonomy operators act on the AQG basis states $|\alpha, k, \mu, \nu\rangle$ in the following way:

$$\hat{h}^{(k_0)}_{e_I}(\mathcal{A})|\alpha, k, \mu, \nu\rangle = \exp\Big(\mathrm{i}\frac{k_0}{2}\mathcal{A}_{e_I}\Big)|\alpha, k, \mu, \nu\rangle = |k_{e_I}+k_0, \mu, \nu\rangle, \quad k_0 \in \mathbb{Z} \tag{6.3}$$

$$\hat{h}^{(\mu_0)}_{v_I}(X)|\alpha, k, \mu, \nu\rangle = \exp\Big(\mathrm{i}\frac{\mu_0}{2}X_{v_I}\Big)|\alpha, k, \mu, \nu\rangle = |\alpha, k, \mu_{v_I}+\mu_0, \nu\rangle, \quad \mu_0 \in \mathbb{R} \tag{6.4}$$

$$\hat{h}^{(\nu_0)}_{v_I}(Y)|\alpha, k, \mu, \nu\rangle = \exp\Big(\mathrm{i}\frac{\nu_0}{2}Y_{v_I}\Big)|\alpha, k, \mu, \nu\rangle = |\alpha, k, \mu, \nu_{v_I}+\nu_0\rangle, \quad \nu_0 \in \mathbb{R}. \tag{6.5}$$

Because in the AQG model there is only one abstract graph α, we will from now on neglect the label for the graph and denote the basis states just by $|k, \mu, \nu_v\rangle$. Note that we can recover the classical expression for the U(1) holonomy from the operator $\hat{h}^{(k_0)}_{e_I}(\mathcal{A})$ by considering semiclassical states that encode in addition to their classical labels in the AQG framework also information about how the abstract graph α is embedded into a given spatial manifold from which an integral along the embedded edges involved in the classical holonomy can be rediscovered, see the results in [59, 60] for the case of the master constraint operator.

The main difference for the fluxes, in turn, is that they can now only act on vertices as there are no embedded edges at hand anymore. Therefore, the elementary flux operator within AQG read

$$\hat{\mathcal{E}}_v|k, \mu, \nu\rangle = \frac{\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2}{2}\frac{k_{e_v}+k_{e_{v^-}}}{2}|k, \mu, \nu\rangle, \tag{6.6}$$

$$\hat{\mathcal{F}}_{x,\mathcal{I}_v}|k, \mu, \nu\rangle = \frac{\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2}{2}\mu_v|k, \mu, \nu\rangle \quad \text{and} \tag{6.7}$$

$$\hat{\mathcal{F}}_{y,\mathcal{I}_v}|k, \mu, \nu\rangle = \frac{\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2}{2}\nu_v|k, \mu, \nu\rangle, \tag{6.8}$$

where k_{e_v} is the at vertex v outgoing edge's U(1)-charge and $k_{e_{v^-}}$ the incoming one's. Note that this trivial continuation from LQG to AQG is possible by choosing the occurring smearing intervals in such a way that they contain one vertex at most: the interval $\mathcal{I}_v$ of (6.7) and (6.8) includes solely vertex v.

The volume operator can be transferred to AQG as straightforwardly as for the basic operators themselves and we get

$$\hat{\mathrm{V}} := \sum_{v\in V(\alpha)} \hat{\mathrm{V}}_v := 4\pi^2 \sum_{v\in V(\alpha)} \sqrt{\left|\hat{\mathcal{E}}_v\right|\left|\hat{\mathcal{F}}_{x,I_v}\right|\left|\hat{\mathcal{F}}_{y,I_v}\right|}, \tag{6.9}$$

with its action on the AQG states (6.2)

$$\hat{\mathrm{V}}_v\,|k,\mu,\nu\rangle = \frac{4\pi^2}{\sqrt{2}}\left(\frac{\beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2}{2}\right)^{\frac{3}{2}} \sqrt{\left|k_{e_v}+k_{e_{v^-}}\right||\mu_v||\nu_v|}\,|k,\mu,\nu\rangle. \tag{6.10}$$

To complete the discussion on the Gauß constraint, we also briefly present how to implement a Gauß constraint operator in AQG. This can be done quite directly as well by considering the LQG Gauß constraint (5.21) that had the form

$$\widehat{G_3} = \frac{1}{\kappa'\beta_{\mathrm{BI}}}\lim_{\epsilon\to 0}\sum_{\mathcal{I}_n\in\mathcal{P}(\epsilon)}\left(\hat{\mathcal{E}}\left(\theta_n+\frac{\epsilon}{2}\right)-\hat{\mathcal{E}}\left(\theta_n-\frac{\epsilon}{2}\right)+\hat{\mathcal{F}}_{\eta,\mathcal{I}_n}\right), \quad \text{with } \theta_n\in\mathcal{I}_n. \tag{5.21}$$

In AQG, we need to implement the operator such that it acts on the vertices of the abstract graph α only and thus we associate $\theta_n - \frac{\epsilon}{2}$ with vertex v^-, the left neighbouring vertex of v, and, accordingly, $\theta_n + \frac{\epsilon}{2}$ with vertex v^+, the right neighbouring vertex of the vertex v. This way, we obtain the following AQG version of the Gauß constraint operator:

$$\begin{aligned}\widehat{G_3}|k,\mu,\nu\rangle &= \frac{1}{\kappa'\beta_{\mathrm{BI}}}\sum_{v\in V(\alpha)}\left(\hat{\mathcal{E}}_{v^+}-\hat{\mathcal{E}}_{v^-}+\hat{\mathcal{F}}_{\eta,\mathcal{I}_v}\right)|k,\mu,\nu\rangle \\ &= \frac{{\ell_{\mathrm{P}}}^2}{\kappa'}\sum_{v\in V(\alpha)}\left(\frac{k_{e_{v^+}}+k_{e_v}-k_{e_{v^-}}-k_{e_{v^{--}}}}{4}+\lambda_v\right)|k,\mu,\nu\rangle,\end{aligned} \tag{6.11}$$

where v^{--} denotes the second vertex to the left of v and we also had to insert the AQG version of the flux conjugate to η:

$$\mathcal{F}_{\eta,e_v}|k,\mu,\nu,\lambda\rangle = \beta_{\mathrm{BI}}{\ell_{\mathrm{P}}}^2\lambda_v|k,\mu,\nu,\lambda\rangle. \tag{6.12}$$

In contrast to the interval $\mathcal{I}_n$ in LQG before, the edge e_v in AQG can only contain one vertex at most, so there is only one contribution within the action of $\mathcal{F}_{\eta,e_v}$. The action of the Gauß constraint on the basis states $|k,\mu,\nu,\lambda\rangle$, in turn, does differ more from its LQG counterpart because for the part involving the flux operators $\hat{\mathcal{E}}$ here the two neighbouring vertices of v are involved. The solution of the AQG Gauss constraint being the equivalent to (5.23) in LQG then reads

$$\lambda_v = -\frac{k_{e_{v+}} + k_{e_v} - k_{e_{v-}} - k_{e_{v--}}}{4} \ , \quad \forall\, v. \tag{6.13}$$

We see that solving λ_v to obtain solutions to the Gauß constraint does also constrain k_{e_v}. In contrast to the LQG case where only the charges of the neighbouring edges of v were involved, we now have a condition depending on the two after next neighbouring ones as well. And without contributions from same edges adding up, as it was the case in LQG, the denominator remains to be 4. This finishes the considerations on the Gauß constraint and we close with the remark that for the work at hand, the Gauß constraint will be solved on the classical level.

6.2 Dynamics of the model with polarised $\mathbb{T}^3$ Gowdy symmetry in AQG

In the following subsection, we will briefly discuss how the physical Hamiltonian operator that was so far quantised in reduced LQG can be implemented in the AQG Gowdy quantum model.

6.2.1 Quantisation of the Euclidean part of the physical Hamiltonian within AQG

We can now straightforwardly transfer the Euclidean part of the physical Hamiltonian operator in (5.65) to AQG by means of the previously stated AQG holonomy operators (6.3), (6.4) and (6.5) as well as the volume operator (6.9). For this purpose, we define the following class of operators $\hat{\mathrm{O}}^{\theta/x/y}_{r,v}$ for $r \in \mathbb{R}, v \in V(\alpha)$ according to

$$\hat{\mathrm{O}}^{\theta}_{r,v} := \cos\frac{\mathcal{A}_{e_v}}{2}\,\hat{\mathrm{V}}^r_v \sin\frac{\mathcal{A}_{e_v}}{2} - \sin\frac{\mathcal{A}_{e_v}}{2}\,\hat{\mathrm{V}}^r_v \cos\frac{\mathcal{A}_{e_v}}{2}, \tag{6.14}$$

$$\hat{\mathrm{O}}^{x}_{r,v} := \cos\frac{X_v}{2}\,\hat{\mathrm{V}}^r_v \sin\frac{X_v}{2} - \sin\frac{X_v}{2}\,\hat{\mathrm{V}}^r_v \cos\frac{X_v}{2} \quad \text{and} \tag{6.15}$$

$$\hat{\mathrm{O}}^{y}_{r,v} := \cos\frac{Y_v}{2}\,\hat{\mathrm{V}}^r_v \sin\frac{Y_v}{2} - \sin\frac{Y_v}{2}\,\hat{\mathrm{V}}^r_v \cos\frac{Y_v}{2}, \tag{6.16}$$

where we used the decomposition of the holonomies into sines and cosines (equations (5.24), (5.25) and (5.26)) offering an alternative, more concise description of the final operator. Now we can substitute the LQG expression involved in the first part of the Euclidean part in (5.55) by the following AQG analogue:

$$\mathrm{tr}\Big(\Big(\hat{h}_x\hat{h}_y\hat{h}_x{}^{-1}\hat{h}_y{}^{-1} - \hat{h}_y\hat{h}_x\hat{h}_y{}^{-1}\hat{h}_x{}^{-1}\Big)\hat{h}_\theta\Big[\hat{h}_\theta{}^{-1}, \hat{\mathrm{V}}_v\Big]\Big) \overset{\mathrm{AQG}}{\longmapsto} -2\sin X_v \sin Y_v \hat{\mathrm{O}}^{\theta}_{1,v}. \tag{6.17}$$

The second and third part of the Euclidean part of the physical Hamiltonian shown in (5.63) and (5.64) entail similar terms with shifted holonomies. Hence, their AQG expressions are of the following form

$$\mathrm{tr}\Big(\Big(\hat{h}_y\hat{h}_\theta\hat{h}_{y,\xi}{}^{-1}\hat{h}_\theta{}^{-1} - \hat{h}_\theta\hat{h}_{y,\xi}\hat{h}_\theta{}^{-1}\hat{h}_y{}^{-1}\Big)\hat{h}_x\Big[\hat{h}_x{}^{-1}, \hat{\mathrm{V}}_v\Big]\Big) \overset{\mathrm{AQG}}{\longmapsto} -4\sin\frac{Y_{v_\xi}}{2}\cos\frac{Y_v}{2}\sin\mathcal{A}_{e_v}\hat{\mathrm{O}}^{x}_{1,v} \tag{6.18}$$

$$\mathrm{tr}\Big(\Big(\hat{h}_\theta\hat{h}_{x,\xi}\hat{h}_\theta{}^{-1}\hat{h}_x{}^{-1} - \hat{h}_x\hat{h}_\theta\hat{h}_{x,\xi}{}^{-1}\hat{h}_\theta{}^{-1}\Big)\hat{h}_y\Big[\hat{h}_y{}^{-1}, \hat{\mathrm{V}}_v\Big]\Big) \overset{\mathrm{AQG}}{\longmapsto} -4\sin\frac{X_{v_\xi}}{2}\cos\frac{X_v}{2}\sin\mathcal{A}_{e_v}\hat{\mathrm{O}}^{y}_{1,v} \tag{6.19}$$

Therein, $X_{v_\xi} = X(v_\xi)$ and $Y_{v_\xi} = Y(v_\xi)$, where v_ξ is v^+ for $\xi = 1$ and v^- for $\xi = -1$ denoting the two neighbouring vertices of v to the right and left respectively.

With this, we can write the Euclidean part of the Hamilton operator in AQG in a form that is more concise and allows for a more compact evaluation of the corresponding action on the Gowdy states later:

$$\hat{\mathrm{H}}_{\mathrm{eucl}} = \sum_{v\in V(\alpha)} \hat{\mathrm{H}}_{\mathrm{eucl},v}, \tag{6.20}$$

with

$$\begin{aligned}\hat{\mathrm{H}}_{\mathrm{eucl},v} :=& -\frac{4\mathrm{i}}{\kappa'\ell_{\mathrm{P}}{}^2 k_0\mu_0\nu_0\beta_{\mathrm{BI}}^3}\Bigg[\sin X_v \sin Y_v \hat{\mathrm{O}}^{\theta}_{1,v} + \\ &+\frac{1}{2}\sum_{\xi=\pm1}\bigg(2\sin\frac{Y_{v_\xi}}{2}\cos\frac{Y_v}{2}\sin\mathcal{A}_{e_v}\hat{\mathrm{O}}^{x}_{1,v} + 2\sin\frac{X_{v_\xi}}{2}\cos\frac{X_v}{2}\sin\mathcal{A}_{e_v}\hat{\mathrm{O}}^{y}_{1,v}\bigg)\Bigg].\end{aligned} \tag{6.21}$$

6.2.2 Quantisation of the Lorentzian part of the physical Hamiltonian within AQG

With all the contained quantities depending on holonomies, fluxes or the volume, we can quantise the Lorentzian part of the physical Hamiltonian that was discussed for the case of reduced LQG in 5.2.2 straightforwardly and also directly in the AQG framework. We then obtain for the first part the following expression

$$\hat{\mathrm{H}}^{(1)}_{\mathrm{lor}} = \sum_{v\in V(\alpha)} \hat{\mathrm{H}}^{(1)}_{\mathrm{lor},v}, \tag{6.22}$$

with

$$\hat{\mathrm{H}}^{(1)}_{\mathrm{lor},v} =: -\frac{4\pi^2}{4\kappa'}\left(\frac{-\mathrm{i}}{\hbar}\right)^{3l}\left(\frac{16}{3(\kappa\beta_{\mathrm{BI}})^3 r^3 k_0\mu_0\nu_0}\right)^{l}\left(\hat{\mathcal{E}}_{v^+}-\hat{\mathcal{E}}_{v}\right)^2 \hat{\mathrm{Z}}_{r,v}{}^{l}\Big|_{r=\frac{2}{3}-\frac{1}{3l}}, \tag{6.23}$$

where we introduced

$$\hat{\mathrm{Z}}_{r,v} := \epsilon^{abc}\,\mathrm{tr}\Big(\hat{h}_a\Big[\hat{h}_a{}^{-1},\hat{\mathrm{V}}_v\Big]\hat{h}_b\Big[\hat{h}_b{}^{-1},\hat{\mathrm{V}}_v\Big]\hat{h}_c\Big[\hat{h}_c{}^{-1},\hat{\mathrm{V}}_v\Big]\Big) = -12\hat{\mathrm{O}}^{x}_{r,v}\hat{\mathrm{O}}^{y}_{r,v}\hat{\mathrm{O}}^{\theta}_{r,v} \tag{6.24}$$

as the equivalent of (5.74). In the semiclassical limit here the intervals corresponding to $\mathcal{I}_n$ in the reduced LQG case will be vertex-labelled intervals $\mathcal{I}_v$.

This procedure can now be applied to the second and third part of the Lorentzian part of the Hamiltonian, (5.41) and (5.42), that also act on the vertices only and thus we just present the operators for the individual vertices v. As the second part contains derivatives of E^x and E^y, the according fluxes $\hat{\mathcal{F}}_{x,\mathcal{I}}$ and $\hat{\mathcal{F}}_{y,\mathcal{I}}$ will appear. Ultimately, the results read

$$\hat{\mathrm{H}}^{(2)}_{\mathrm{lor},v} = \tfrac{4\pi^2}{4\kappa'}\left(\tfrac{-\mathrm{i}}{\hbar}\right)^{3l}\left(\tfrac{16}{3(\kappa\beta_{\mathrm{BI}}r_2)^3 k_0\mu_0\nu_0}\right)^{l}\hat{\mathcal{E}}_v{}^{4}\left(\hat{\mathcal{F}}_{x,\mathcal{I}_v}\hat{\mathcal{F}}_{y,\mathcal{I}_{v^+}}-\hat{\mathcal{F}}_{y,\mathcal{I}_v}\hat{\mathcal{F}}_{x,\mathcal{I}_{v^+}}\right)^2\hat{\mathrm{Z}}_{r_2,v}{}^{l}\Big|_{r_2=\frac{2}{3}-\frac{5}{3l}} \quad \text{and} \tag{6.25}$$

$$\hat{\mathrm{H}}^{(3)}_{\mathrm{lor},v} = \tfrac{4\pi^2}{\kappa'}\left(\tfrac{-\mathrm{i}}{\hbar}\right)^{3l}\left(\tfrac{16}{3(\kappa\beta_{\mathrm{BI}}r)^3 k_0\mu_0\nu_0}\right)^{l}\left(\hat{\mathcal{E}}_{v^+}\left(\hat{\mathcal{E}}_{v^{++}}-\hat{\mathcal{E}}_{v^+}\right)\hat{\mathrm{Z}}_{r,v^+}{}^{l}-\hat{\mathcal{E}}_{v}\left(\hat{\mathcal{E}}_{v^+}-\hat{\mathcal{E}}_{v}\right)\hat{\mathrm{Z}}_{r,v}{}^{l}\right)\Big|_{r=\frac{2}{3}-\frac{1}{3l}}. \tag{6.26}$$

In accordance with [198, 200, 201], the second part was quantised in a different manner than in [164]. While the latter introduced the inverse flux to cope with the denominators

E^x and E^y appearing in (5.41), the alternative route leading to the quantisation above uses

$$\frac{1}{E^x} = \frac{E^y\mathcal{E}}{\left(\sqrt{\det E}\right)^2} \quad \text{and} \quad \frac{1}{E^y} = \frac{E^x\mathcal{E}}{\left(\sqrt{\det E}\right)^2}, \tag{6.27}$$

leading to the volume squared as denominator. Therefore, we can insert a new $(1)^l$ for which

$$r_2 = \frac{2}{3} - \frac{5}{3l} \tag{6.28}$$

holds and resolve the inverse volume squared in the same manner as for the inverse volume before. Lastly, we set $\mu_0 = 1 = \nu_0$.

Finally, the physical Hamiltonian operator now reads altogether

$$\hat{\mathrm{H}}_{\mathrm{phys}} = \sum_{v\in V(\alpha)} \hat{\mathrm{H}}_{\mathrm{phys,v}} = \frac{1}{2}\sum_{v\in V(\alpha)} \left(\hat{\mathrm{H}}_{\mathrm{eucl},v} + (\hat{\mathrm{H}}_{\mathrm{eucl},v})^\dagger + \hat{\mathrm{H}}_{\mathrm{lor},v} + (\hat{\mathrm{H}}_{\mathrm{lor},v})^\dagger\right), \tag{6.29}$$

with

$$\begin{aligned}
\hat{\mathrm{H}}_{\mathrm{eucl}} + \hat{\mathrm{H}}_{\mathrm{lor}} &= \hat{\mathrm{H}}_{\mathrm{eucl}} + \hat{\mathrm{H}}^{(1)}_{\mathrm{lor}} + \hat{\mathrm{H}}^{(2)}_{\mathrm{lor}} + \hat{\mathrm{H}}^{(3)}_{\mathrm{lor}} = \sum_{v\in V(\alpha)} \left(\hat{\mathrm{H}}_{\mathrm{eucl},v} + \hat{\mathrm{H}}^{(1)}_{\mathrm{lor},v} + \hat{\mathrm{H}}^{(2)}_{\mathrm{lor},v} + \hat{\mathrm{H}}^{(3)}_{\mathrm{lor},v}\right) \\
&= \sum_{v\in V(\alpha)} \Bigg\{ - \frac{4\mathrm{i}}{\kappa' {\ell_{\mathrm{P}}}^2 k_0 \mu_0 \nu_0 \beta_{\mathrm{BI}}^3} \Bigg[\sin X_v \sin Y_v \hat{\mathrm{O}}^{\theta}_{1,v} + \\
&\quad + \frac{1}{2}\sum_{\xi=\pm 1} \left(2\sin\tfrac{Y_{v_\xi}}{2} \cos\tfrac{Y_v}{2} \sin\mathcal{A}_{e_v} \hat{\mathrm{O}}^{x}_{1,v} + 2\sin\tfrac{X_{v_\xi}}{2}\cos\tfrac{X_v}{2}\sin\mathcal{A}_{e_v}\hat{\mathrm{O}}^{y}_{1,v}\right)\Bigg] \\
&\quad - \tfrac{4\pi^2}{4\kappa'}\left(\tfrac{16\mathrm{i}}{3{\ell_{\mathrm{P}}}^6 \beta_{\mathrm{BI}}^3 r^3 k_0\mu_0\nu_0}\right)^l \left(\hat{\mathcal{E}}_{v^+} - \hat{\mathcal{E}}_v\right)^2 {\hat{\mathrm{Z}}_{r,v}}^{\,l}\Big|_{r=\frac{2}{3}-\frac{1}{3l}} \\
&\quad + \tfrac{4\pi^2}{4\kappa'}\left(\tfrac{16\mathrm{i}}{3{\ell_{\mathrm{P}}}^6 \beta_{\mathrm{BI}}^3 r_2^3 k_0\mu_0\nu_0}\right)^l {\hat{\mathcal{E}}_v}^{\,4}\left(\hat{\mathcal{F}}_{x,\mathcal{I}_v}\hat{\mathcal{F}}_{y,\mathcal{I}_{v^+}} - \hat{\mathcal{F}}_{y,\mathcal{I}_v}\hat{\mathcal{F}}_{x,\mathcal{I}_{v^+}}\right)^2 {\hat{\mathrm{Z}}_{r_2,I}}^{\,l}\Big|_{r_2=\frac{2}{3}-\frac{5}{3l}} \\
&\quad + \tfrac{4\pi^2}{\kappa'}\left(\tfrac{16\mathrm{i}}{3{\ell_{\mathrm{P}}}^6 \beta_{\mathrm{BI}}^3 r^3 k_0\mu_0\nu_0}\right)^l \left(\hat{\mathcal{E}}_{v^+}\left(\hat{\mathcal{E}}_{v^{++}} - \hat{\mathcal{E}}_{v^+}\right){\hat{\mathrm{Z}}_{r,v^+}}^{\,l} - \hat{\mathcal{E}}_v\left(\hat{\mathcal{E}}_{v^+} - \hat{\mathcal{E}}_v\right){\hat{\mathrm{Z}}_{r,v}}^{\,l}\right)\Big|_{r=\frac{2}{3}-\frac{1}{3l}}\Bigg\}.
\end{aligned} \tag{6.30}$$

Comparing the results for the final physical Hamiltonian operator in reduced LQG in (5.78) and for AQG in (6.29), they reflect again the underlying difference of the way graph-preserving operators are implemented. For reduced LQG, these involve a sum over all possible embedded finite graphs Γ and the operator preserves each graph Hilbert space $\mathcal{H}_\Gamma$ separately, whereas in AQG the operator involves a sum over the vertices of the abstract infinite graph α. This finishes the discussion on the quantisation of the physical Hamiltonian of the Gowdy model in the AQG framework.

Chapter 7

First steps in applying the AQG Gowdy model

In this chapter, we present first steps in applying the AQG Gowdy model derived in the former chapters of this part. In particular, we want to discuss the Schrödinger-like equation that encodes the dynamics of the quantum model. For this purpose, we compute the action of the physical Hamiltonian $\hat{\mathrm{H}}_{\mathrm{phys}}$ on the basis states and due to its complexity we will discuss the individual parts of the Euclidean and Lorentzian contributions to $\hat{\mathrm{H}}_{\mathrm{phys}}$ separately.

7.1 The Schrödinger-like equation for the AQG Gowdy model

Given the physical Hamiltonian operator in the AQG Gowdy model $\hat{\mathrm{H}}_{\mathrm{phys}}$ in (6.29), we can take it as the starting point to derive the corresponding Schrödinger-like equation encoding the dynamics of the model. For simplicity, we will restrict our discussion to the case where we choose $\xi = 1$ only and neglect the contribution coming from $\xi = -1$ in the sum in (6.30) in the Euclidean part because such a restriction will not be very relevant for the applications discussed in this section but simplifies the individual formulae. To ensure that the semiclassical limit is still correct, we need to add an additional factor of 2 here that cancels the factor of $\frac{1}{2}$ in front of the sum over ξ in (6.30). Carried over to the reduced LQG case, such a restriction can also be understood as a slightly different regularisation of the operator where the shifted holonomies involved act only to the right hand side of the vertex v but not to the left. As discussed above, in the definition of $\hat{\mathrm{H}}_{\mathrm{phys}}$ we choose the symmetric combination of the individual parts, i.e. we have

$$\hat{\mathrm{H}}_{\mathrm{phys}} = \frac{1}{2}\Big(\hat{\mathrm{H}}_{\mathrm{eucl}} + \hat{\mathrm{H}}_{\mathrm{eucl}}{}^{\dagger}\Big) + \hat{\mathrm{H}}_{\mathrm{lor}}, \tag{7.1}$$

where we already used that $\hat{\mathrm{H}}_{\mathrm{lor}}$ will turn out to be symmetric and thus we only need to consider the symmetric combination of $\hat{\mathrm{H}}_{\mathrm{eucl}}$. We can directly see this by calculating the adjoint version of $\hat{\mathrm{H}}_{\mathrm{eucl}}$. While the contained trigonometric functions $\sin X_v$, $\cos X_v$, $\sin Y_v$ etc. are self-adjoint due to

$$(\sin X_v)^{\dagger} = \left(\frac{1}{2\mathrm{i}}\big(\mathrm{e}^{\mathrm{i}X_v} - \mathrm{e}^{-\mathrm{i}X_v}\big)\right)^{\dagger} = -\frac{1}{2\mathrm{i}}\big(\mathrm{e}^{-\mathrm{i}X_v} - \mathrm{e}^{\mathrm{i}X_v}\big) = \sin X_v, \tag{7.2}$$

the class of operators $\hat{\mathrm{O}}^{\theta/x/y}_{r,v}$ is indeed not. Rewriting (6.15) as

$$\hat{\mathrm{O}}^{x}_{r,v} = \cos\frac{X_v}{2}\,\hat{\mathrm{V}}^{r}_{v}\sin\frac{X_v}{2} - \sin\frac{X_v}{2}\,\hat{\mathrm{V}}^{r}_{v}\cos\frac{X_v}{2} = \frac{1}{2\mathrm{i}}\Big(\mathrm{e}^{-\frac{\mathrm{i}}{2}X_v}\,\hat{\mathrm{V}}^{r}_{v}\,\mathrm{e}^{\frac{i}{2}X_v} - \mathrm{e}^{\frac{\mathrm{i}}{2}X_v}\,\hat{\mathrm{V}}^{r}_{v}\,\mathrm{e}^{-\frac{i}{2}X_v}\Big), \tag{7.3}$$

which we will also later use to compute the action of the physical Hamilton operator on the basis states, we obtain

$$\Big(\hat{\mathrm{O}}^{x}_{r,v}\Big)^{\dagger} = -\frac{1}{2\mathrm{i}}\Big(\mathrm{e}^{-\frac{\mathrm{i}}{2}X_v}\,\hat{\mathrm{V}}^{r}_{v}\,\mathrm{e}^{\frac{i}{2}X_v} - \mathrm{e}^{\frac{\mathrm{i}}{2}X_v}\,\hat{\mathrm{V}}^{r}_{v}\,\mathrm{e}^{-\frac{i}{2}X_v}\Big) = -\hat{\mathrm{O}}^{x}_{r,v}. \tag{7.4}$$

Altogether, this results in

$$\begin{aligned}(\hat{\mathrm{H}}_{\mathrm{eucl},v})^{\dagger} = -\frac{4\mathrm{i}}{\kappa'\ell_{\mathrm{P}}{}^{2}k_0\mu_0\nu_0\beta_{\mathrm{BI}}^{3}}\Bigg(&\hat{\mathrm{O}}^{\theta}_{1,v}\sin X_v\sin Y_v + 2\hat{\mathrm{O}}^{x}_{1,v}\sin\frac{Y_{v+}}{2}\cos\frac{Y_v}{2}\sin\mathcal{A}_{e_v} + \\ &+ 2\hat{\mathrm{O}}^{y}_{1,v}\sin\frac{X_{v+}}{2}\cos\frac{X_v}{2}\sin\mathcal{A}_{e_v}\Bigg).\end{aligned} \tag{7.5}$$

It is then straightforward to see that this acts differently on the states $|k,\mu,\nu\rangle$ than $\hat{\mathrm{H}}_{\mathrm{eucl},v}$ does (cf. (6.22)): The trigonometric functions, which act first in the adjoint version, increase or decrease the charges (cf. (7.2)) and the volume operator within the class of operators $\hat{\mathrm{O}}^{\theta/x/y}_{1,v}$ then reads out different charges than the non-adjoint $\hat{\mathrm{H}}_{\mathrm{eucl},v}$ does.

The increasingly long expression for $\hat{\mathrm{H}}_{\mathrm{phys}}$ can, however, also be reduced by one of its contributions. Namely, via the action[1] of $\hat{\mathrm{H}}^{(3)}_{\mathrm{lor}}$ on the basis states $|k,\mu,\nu\rangle$

$$\begin{aligned}\hat{\mathrm{H}}^{(3)}_{\mathrm{lor}}|k,\mu,\nu\rangle &= \sum_{v\in V(\alpha)} \hat{\mathrm{H}}^{(3)}_{\mathrm{lor},v}\,|k,\mu,\nu\rangle = \sum_{v\in V(\alpha)} \frac{4\pi^2\ell_{\mathrm{P}}\sqrt{\beta_{\mathrm{BI}}}}{4\kappa'}\left(\frac{1}{2r^3k_0\mu_0\nu_0}\right)^l\Big|_{r=\frac{2}{3}-\frac{1}{3l}}\cdot\\ &\cdot\Bigg\{\big(k_{e_{v^+}}+k_{e_v}\big)\big(k_{e_{v^{++}}}-k_{e_v}\big)\cdot\Big[\Big(|\mu_{v^+}+1|^{\frac{r}{2}}-|\mu_{v^+}-1|^{\frac{r}{2}}\Big)\Big(|\nu_{v^+}+1|^{\frac{r}{2}}-|\nu_{v^+}-1|^{\frac{r}{2}}\Big)\\ &\cdot\Big(\big|k_{e_{v^+}}+k_{e_v}+1\big|^{\frac{r}{2}}-\big|k_{e_{v^+}}+k_{e_v}-1\big|^{\frac{r}{2}}\Big)|\mu_{v^+}|^r|\nu_{v^+}|^r\big|k_{e_{v^+}}+k_{e_v}\big|^r\Big]^l-\\ &-\big(k_{e_v}+k_{e_{v^-}}\big)\big(k_{e_{v^+}}-k_{e_{v^-}}\big)\cdot\Big[\Big(|\mu_v+1|^{\frac{r}{2}}-|\mu_v-1|^{\frac{r}{2}}\Big)\Big(|\nu_v+1|^{\frac{r}{2}}-|\nu_v-1|^{\frac{r}{2}}\Big)\\ &\cdot\Big(\big|k_{e_v}+k_{e_{v^-}}+1\big|^{\frac{r}{2}}-\big|k_{e_v}+k_{e_{v^-}}-1\big|^{\frac{r}{2}}\Big)|\mu_v|^r|\nu_v|^r\big|k_{e_v}+k_{e_{v^-}}\big|^r\Big]^l\Bigg\}|k,\mu,\nu\rangle,\end{aligned}\tag{7.6}$$

we conclude that this expression vanishes: The minuend and the subtrahend of the difference within the curly brackets are structurally the same and only differ by the contained charges' indices via $v^{++}\mapsto v^+, v^+\mapsto v$ and $v\mapsto v^-$, meaning that each vertex is mapped to its left neighbouring one. By taking the sum over all $v\in V(\alpha)$, i.e. the sum over all vertices of the graph α, this becomes a telescope series. Reminding ourselves that we implemented boundary conditions such that we mimic also in the AQG case the situation to sum along a closed circle as it is done in the reduced LQG model, we realise that the first and last contribution of the series then are the same which means as a result that the telescope series sums up to zero. Putting it into formulae, let us write this in compact form as

$$(7.6) =: \sum_{v\in V(\alpha)}\Big(h^{(3)}_{\mathrm{lor},v^+}-h^{(3)}_{\mathrm{lor},v}\Big)|k,\mu,\nu\rangle,\tag{7.7}$$

where $h^{(3)}_{\mathrm{lor},v^+}$ represents the respective minuends within the curly bracket of (7.6) and $h^{(3)}_{\mathrm{lor},v}$ the corresponding subtrahends. Now, assuming the abstract graph has N edges with non-trivial representations on the edges then via the difference within the summands of the series in (7.7), all contributions but the ones for the first vertex v_1 and the last one v_{N+1} appear twice and in particular with different signs. Hence,

$$(7.7) = h^{(3)}_{\mathrm{lor},v_{N+1}}-h^{(3)}_{\mathrm{lor},v_1}\tag{7.8}$$

[1] We describe the action of the main components on the basis states in more detail within the next subsection.

and as the definition of the abstract Gowdy graph involved periodic boundary conditions such that the vertices v_{N+1} and v_1 are identified, this results in the contribution of $\hat{\mathrm{H}}^{(3)}_{\mathrm{lor}}$ to vanish. This means that the final physical Hamiltonian reads

$$\hat{\mathrm{H}}_{\mathrm{phys}} = \frac{1}{2}\Big(\hat{\mathrm{H}}_{\mathrm{eucl}} + (\hat{\mathrm{H}}_{\mathrm{eucl}})^{\dagger}\Big) + \hat{\mathrm{H}}^{(1)}_{\mathrm{lor}} + \hat{\mathrm{H}}^{(2)}_{\mathrm{lor}} \,. \tag{7.9}$$

7.1.1 Action of $\hat{\mathrm{H}}_{\mathrm{phys}}$'s main components on the basis states $|k, \mu, \nu\rangle$

In order to make future calculations easier and provide a concise overview, we will now state how the main components of $\hat{\mathrm{H}}_{\mathrm{phys}}$ act on the basis states $|k, \mu, \nu\rangle$. We start with the trigonometric functions

$$\sin \mathcal{A}_{e_I}|k,\mu,\nu\rangle = \frac{1}{2\mathrm{i}}(|k_{e_v}+2,\mu,\nu\rangle - |k_{e_v}-2,\mu,\nu\rangle), \tag{7.10}$$

$$\cos \mathcal{A}_{e_I}|k,\mu,\nu\rangle = \frac{1}{2}(|k_{e_v}+2,\mu,\nu\rangle + |k_{e_v}-2,\mu,\nu\rangle), \tag{7.11}$$

$$\sin X_v|k,\mu,\nu\rangle = \frac{1}{2\mathrm{i}}(|k,\mu_v+2,\nu\rangle - |k,\mu_v-2,\nu\rangle), \tag{7.12}$$

$$\cos X_v|k,\mu,\nu\rangle = \frac{1}{2}(|k,\mu_v+2,\nu\rangle + |k,\mu_v-2,\nu\rangle), \tag{7.13}$$

$$\sin Y_v|k,\mu,\nu\rangle = \frac{1}{2\mathrm{i}}(|k,\mu,\nu_v+2\rangle - |k,\mu,\nu_v-2\rangle) \quad \text{and} \tag{7.14}$$

$$\cos Y_v|k,\mu,\nu\rangle = \frac{1}{2}(|k,\mu,\nu_v+2\rangle + |k,\mu,\nu_v-2\rangle) \tag{7.15}$$

that we used instead of the actual holonomies. To have a complete list, we also recap the fluxes' actions

$$\hat{\mathcal{E}}_v|k,\mu,\nu\rangle = \frac{\beta_{\mathrm{BI}}\ell_{\mathrm{P}}{}^2}{2}\frac{k_{e_v}-k_{e_{v-}}}{2}|k,\mu,\nu\rangle \tag{6.6}$$

$$\hat{\mathcal{F}}_{x,\mathcal{I}_v}|k,\mu,\nu\rangle = \frac{\beta_{\mathrm{BI}}\ell_{\mathrm{P}}{}^2}{2}\mu_v|k,\mu,\nu\rangle \quad \text{and} \tag{6.7}$$

$$\hat{\mathcal{F}}_{y,\mathcal{I}_v}|k,\mu,\nu\rangle = \frac{\beta_{\mathrm{BI}}\ell_{\mathrm{P}}{}^2}{2}\nu_v|k,\mu,\nu\rangle. \tag{6.8}$$

Then, for the class of the $\hat{\mathrm{O}}^{\theta/x/y}_{r,v}$ operators, we get

$$\hat{\mathrm{O}}^{\theta}_{r,v}|k,\mu,\nu\rangle = \frac{1}{2\mathrm{i}}\left(\frac{\ell_{\mathrm{P}}{}^3\beta_{\mathrm{BI}}^{\frac{3}{2}}}{4}\right)^r\left(\left|k_{e_v}+1+k_{e_{v}-}\right|^{\frac{r}{2}}-\left|k_{e_v}-1+k_{e_{v}-}\right|^{\frac{r}{2}}\right)|\mu_v|^{\frac{r}{2}}|\nu_v|^{\frac{r}{2}}|k,\mu,\nu\rangle, \tag{7.16}$$

$$\hat{\mathrm{O}}^{x}_{r,v}|k,\mu,\nu\rangle = \frac{1}{2\mathrm{i}}\left(\frac{\ell_{\mathrm{P}}{}^3\beta_{\mathrm{BI}}^{\frac{3}{2}}}{4}\right)^r\left|k_{e_v}+k_{e_{v}-}\right|^{\frac{r}{2}}\left(|\mu_v+1|^{\frac{r}{2}}-|\mu_v-1|^{\frac{r}{2}}\right)|\nu_v|^{\frac{r}{2}}|k,\mu,\nu\rangle \quad \text{and} \tag{7.17}$$

$$\hat{\mathrm{O}}^{y}_{r,v}|k,\mu,\nu\rangle = \frac{1}{2\mathrm{i}}\left(\frac{\ell_{\mathrm{P}}{}^3\beta_{\mathrm{BI}}^{\frac{3}{2}}}{4}\right)^r\left|k_{e_v}+k_{e_{v}-}\right|^{\frac{r}{2}}|\mu_v|^{\frac{r}{2}}\left(|\nu_v+1|^{\frac{r}{2}}-|\nu_v-1|^{\frac{r}{2}}\right)|k,\mu,\nu\rangle, \tag{7.18}$$

where we used the action of the volume operator according to (6.10). And lastly,

$$\begin{aligned}\hat{\mathrm{Z}}_{r,v}{}^l|k,\mu,\nu\rangle = (-12)^l\left(\frac{1}{2\mathrm{i}}\left(\frac{\ell_{\mathrm{P}}{}^3\beta_{\mathrm{BI}}^{3/2}}{4}\right)^r\right)^{3l}\Big[\left(\left|k_{e_v}+1+k_{e_{v}-}\right|^{\frac{r}{2}}-\left|k_{e_v}-1+k_{e_{v}-}\right|^{\frac{r}{2}}\right)\cdot\\ \cdot\left(|\mu_v+1|^{\frac{r}{2}}-|\mu_v-1|^{\frac{r}{2}}\right)\left(|\nu_v+1|^{\frac{r}{2}}-|\nu_v-1|^{\frac{r}{2}}\right)\left|k_{e_v}+k_{e_{v}-}\right|^r|\mu_v|^r|\nu_v|^r\Big]^l|k,\mu,\nu\rangle.\end{aligned} \tag{7.19}$$

The individual action of these operators will be used in the next subsection where we discuss Gowdy states in the AQG framwork in more detail.

7.1.2 Gowdy states in the AQG model

We briefly discussed at the beginning of Chapter 6 how the symmetry reduced Gowdy model can be carried over to the AQG framework. Because the physical Hamiltonian operator $\hat{\mathrm{H}}_{\mathrm{phys}}$ also involves the adjoint $(\hat{\mathrm{H}}_{\mathrm{eucl}})^\dagger$, we need to discuss in more detail how we can perform an adaption of the AQG-graph we consider. Due to the appearance of $(\hat{\mathrm{H}}_{\mathrm{eucl}})^\dagger$ within $\hat{\mathrm{H}}_{\mathrm{phys}}$ and its action on $|k,\mu,\nu\rangle$, we allow only those states in the model that have only a finite number of the infinite number of edges with non-trivial U(1)-charges k_{e_v}, the remaining one carry trivial representations. The action of the physical Hamilton operator $\hat{\mathrm{H}}_{\mathrm{phys}}$ of (6.30) on trivially charged vertices vanishes as there is always an operator of the class $\hat{\mathrm{O}}^{\theta/x/y}_{r,v}$ acting first. Taking a look at their action on the basis states ((7.16), (7.17) and (7.18)), we see that they vanish on trivially charged vertices — cf. (6.10) to see that it suffices that one of $k_{e_v}=-k_{e_{v}-}$, $\mu_v=0$ or $\nu_v=0$ holds.

This changes for the action of the adjoint operator $(\hat{\mathrm{H}}_{\mathrm{eucl}})^{\dagger}$, (7.5). Its first term acts with $\sin X_v \sin Y_v$ before $\hat{\mathrm{O}}^{\theta}_{1,v}$, thereby charging the two previously neutral charges μ_v and ν_v. Hence, $\hat{\mathrm{O}}^{\theta}_{1,v}$ returns a non-zero value that is, i.a., $\sim \left|k_{e_v} + 1 + k_{e_{v^-}}\right|^{\frac{r}{2}} - \left|k_{e_v} - 1 + k_{e_{v^-}}\right|^{\frac{r}{2}}$. This still vanishes for vertices v with trivially charged neighbouring edges $e_{v_{I-1}}$ and e_{v_I}. But taking a look at Figure 6.1, we see that vertex v_{N+1} — which is trivially charged by means of $k_{e_{v_{N+1}}} = 0$, $\mu_{v_{N+1}} = 0$ and $\nu_{v_{N+1}} = 0$ — has also e_{v_N} as neighbouring edge for which, i.a., $k_{e_{v_N}} \neq 0$ holds. Therefore, $(\hat{\mathrm{H}}_{\mathrm{eucl},v})^{\dagger}|k,\mu,\nu\rangle$ does not vanish for $v_I = v_{N+1}$. However, we can fix this by fulfilling the condition $k_{e_v} = -k_{e_{v^-}}$ to obtain a zero eigenvalue and set $k_{e_{v_{N+1}}} = -k_{e_{v_N}}$. Consequently, to have all the following trivially charged vertices to have vanishing contributions as well, we need to set $k_{e_{v_{N+2}}} = -k_{e_{v_{N+1}}} = k_{e_{v_N}}$ and so forth, i.e. all edges $e_I, I > N$, are charged with $k_{e_v} \cdot (-1)^{I-N}$. Figure 7.1 illustrates these new states and Figure 7.2 does so for an embedded graph. The embedding is done by creating two additional, trivially charged vertices v' and v'' between v_N and v_1 and mapping all edges that are charged with $-k_N$ to the edge between v' and v'', while all edges that are charged with $k_{e_{v_N}}$ are mapped to the edge between v'' and v_1. Note that the latter take over the role of the previously $k_{e_{v_N}}$-charged edge e_0 to the left of v_1 (cf. Fig. 7.1).

Note that all the above is not the case for the other two contributions of $(\hat{\mathrm{H}}_{\mathrm{eucl}})^{\dagger}$: Besides $\sin \mathcal{A}_{e_{v_I}}$, only trigonometric functions of either X_v *or* Y_v act before $\hat{\mathrm{O}}^{y}_{1,v}$ or $\hat{\mathrm{O}}^{x}_{1,v}$ respectively. Hence, via their action according to (7.18) and (7.17), $\hat{\mathrm{O}}^{y}_{1,v}$ contributes with a value $\sim |\nu_v + 1|^{\frac{r}{2}} - |\nu_v - 1|^{\frac{r}{2}}$, where the charge $\nu_v = 0$ is still the initial neutral one. The same holds for $\hat{\mathrm{O}}^{x}_{1,v}$ and $\mu_v = 0$ and we do not need to perform further adaptions.

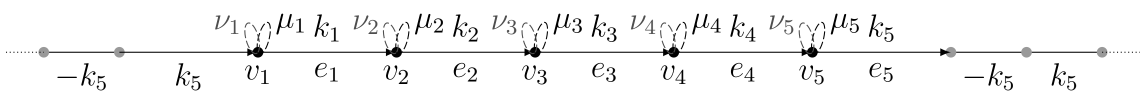


Figure 7.1: The abstract infinite AQG-graph of Figure 6.1, now also ensuring trivially charged vertices not to contribute via the action of $(\hat{\mathrm{H}}_{\mathrm{eucl}})^{\dagger}$ — as guaranteed by alternating charges $\pm k_5$ on the previously uncharged edges $e_I, I > 5$. To keep the notation more compact, we used $k_{e_{v_I}} =: k_I, \mu_{v_I} =: \mu_I$ and $\nu_{v_I} =: \nu_I$.

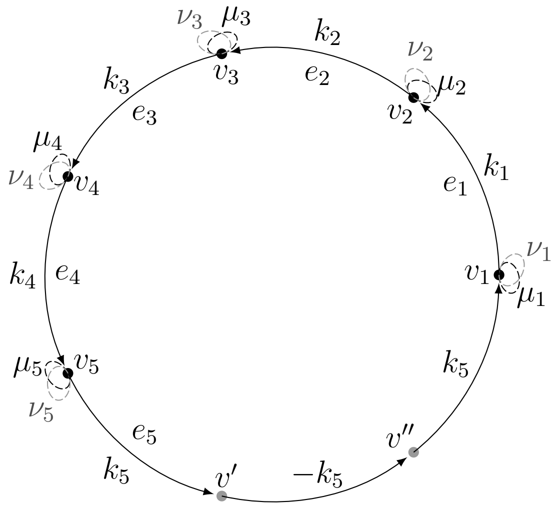


Figure 7.2: An embedding of the abstract infinite AQG-graph of Figure 7.1, which also ensures trivially charged vertices not to contribute via the action of $(\hat{\mathrm{H}}_{\mathrm{eucl}})^\dagger$ — as guaranteed by the new uncharged vertices v' and v'' and the new k_5- and $-k_5$-charged edges around them, compared to Fig. 5.1. To keep the notation more compact we used $k_{e_{v_I}} =: k_I, \mu_{v_I} =: \mu_I$ and $\nu_{v_I} =: \nu_I$.

Having found a suitable form for the basis states $|k, \mu, \nu\rangle$, we can now address the states $|\Psi\rangle(\tau)$ that we will use for writing down an ansatz for the solution of the Schrödinger-like equation of the Gowdy model given by

$$i\hbar\frac{\partial}{\partial\tau}|\Psi(\tau)\rangle = \hat{\mathrm{H}}_{\mathrm{phys}}\,|\Psi(\tau)\rangle \tag{7.20}$$

later on in Section 7.2. For the state $|\Psi(\tau)\rangle$ we use the following separation ansatz:

$$|\Psi\rangle(\tau) = |\varphi(k,\mu,\nu)\rangle|\chi(\tau)\rangle, \tag{7.21}$$

where we put the dependence on the physical time τ completely into $\chi(\tau)$, while that quantity, in turn, does not depend on k_{e_v}, μ_v or ν_v and solely $|\varphi\rangle$ does. Our ansatz for $|\varphi\rangle$ then reads

$$|\varphi\rangle \coloneqq \sum_{k\in\mathbb{Z}^N}\sum_{\mu_v\in m}\sum_{\nu\in n} C_{k,\mu,\nu}|k,\mu,\nu\rangle, \tag{7.22}$$

whose structure we illustrate in the following in more detail along the lines of [198].

In the above, N is the number of vertices and k, μ and ν are multi-labels: $k := (k_{e_{v_1}}, ..., k_{e_{v_N}})$, $\mu := (\mu_{v_1}, ..., \mu_{v_N})$ and $\nu := (\nu_{v_1}, ..., \nu_{v_N})$. Lastly,

$$C_{k,\mu,\nu} := C_{k_{e_{v_1}},...,k_{e_{v_N}},\mu_{v_1},...,\mu_{v_N},\nu_{v_1},...,\nu_{v_N}} \tag{7.23}$$

are coefficients that depend on all k-, μ- and ν-labels. While k takes values in $\mathbb{Z}^N$, the sets $m := m_1 \times ... \times m_N$ and $n := n_1 \times ... \times n_N$ allow slightly more flexibility:

$$m_{v_j} := \{\widetilde{\mu}_{v_j} + p \mid p \in \mathbb{Z}\} \text{ and } n_{v_j} := \{\widetilde{\nu}_{v_j} + p \mid p \in \mathbb{Z}\} \text{ with } \widetilde{\mu}_{v_j}, \widetilde{\nu}_{v_j} \in \mathbb{R} \;\; \forall j \in \{1, ..., N\} \tag{7.24}$$

To motivate this choice, we have a closer look at the point holonomies and take the one of X as an example. Within its expression $\exp\left(\frac{i}{2}\mu_{v_j} X_{v_j}\right)$, $\mu_{v_j} \in \mathbb{R}$ labels the specific irreducible representation of the Bohr compactification $\overline{\mathbb{R}}_{\text{Bohr}}$ for each vertex v_j. The corresponding Hilbert space $\mathcal{H}^X_{v_j} := L_2(\overline{\mathbb{R}}_{\text{Bohr}}, d\mu_{\text{Bohr}})$ consists of square integrable functions f over $\overline{\mathbb{R}}_{\text{Bohr}}$ with respect to its Haar measure $\mathrm{d}\mu_{\text{Bohr}}$. The inner product in this Hilbert space reads

$$\langle f \mid g \rangle := \lim_{R\to\infty} \frac{1}{2R} \int_{-R}^{+R} \mathrm{d}x f(x)^* g(x), \tag{7.25}$$

wherein f^* is the complex conjugate of f. Now, using $\langle x|\mu_{v_j}\rangle := \exp\left(\frac{i}{2}\mu_{v_j} x\right)$, we find the inner product of two basis states to be

$$\langle \mu_{v_j} \mid \mu'_{v_j} \rangle := \lim_{R\to\infty} \frac{1}{2R} \int_{-R}^{+R} \mathrm{d}x \; \mathrm{e}^{\frac{i}{2}(\mu'_{v_j} - \mu_{v_j})} = \delta_{\mu_{v_j}, \mu'_{v_j}}, \tag{7.26}$$

with the Kronecker delta $\delta_{\mu_{v_j}, \mu'_{v_j}}$, and also deduce the completeness relation

$$\sum_{\mu_{v_j} \in m_j} |\mu_{v_j}\rangle\langle\mu_{v_j}| = \mathbb{1}_{\mathcal{H}^X_{v_j}}. \tag{7.27}$$

Therein, $\mu_{v_j} \in m_j$, which is a finite subset of $\mathbb{R}$. And it has to be a finite subset in order for a state

$$\mathcal{H}^X_{v_j} \ni |\phi\rangle = \sum_{\mu_{v_j} \in m_j} c_{\mu_{v_j}} |\mu_{v_j}\rangle, \tag{7.28}$$

with arbitrary coefficients $c_{\mu_{v_j}}$, to be normalisable — i.e. allowing it to be an element of the Hilbert space after all. When it comes to our applications of the Gowdy model, however, we need to fall back on formal states, whose labels can take values in infinite sets. The reason being that some of the operators we have to deal with will map out of an otherwise finite set: While the Lorentzian part of the physical Hamiltonian acts diagonally, we notice the Euclidean part (6.22) to contain the operators

$$\sin\big(X_{v_j}\big) = \frac{1}{2i}\Big(\mathrm{e}^{i\frac{\mu_{v_j}}{2}\cdot 2X_{v_j}} - \mathrm{e}^{-i\frac{\mu_{v_j}}{2}\cdot 2X_{v_j}}\Big) \text{ and } \sin\big(Y_{v_j}\big) = \frac{1}{2i}\Big(\mathrm{e}^{i\frac{\nu_{v_j}}{2}\cdot 2Y_{v_j}} - \mathrm{e}^{-i\frac{\nu_{v_j}}{2}\cdot 2Y_{v_j}}\Big). \tag{7.29}$$

Clearly, those do not act diagonally and with the following operator $\hat{\mathrm{O}}^{\theta}_{1,v}$ in (6.22) acting again diagonally, we do have an overall non-diagonal action. If we now choose the labels of the point holonomies to take values from a finite subset, say $m' = n' = u \times ... \times u$ with $u := \{8, 27, 2022\}$, the above operators of (7.29) will map a value 16 of one of the labels of a state i.a. to the new label $27 + 2 = 29 \notin u$. This problem clearly exists for any choice of finite u. Therefore, we have to choose infinite sets for the labels' values, where the individual elements are separated by steps of ± 1 — note that the physical Hamiltonian (6.22) also contains the above operators with their arguments divided by 2. Without having any constraint on "where" this sequence starts, we can choose an arbitrary value $\widetilde{\mu}_{v_j} \in \mathbb{R}$ to construct the set $m_{v_j} := \{\widetilde{\mu}_{v_j} + p \mid p \in \mathbb{Z}\} \ni \mu_{v_j}$ and similarly for all other vertices. For symmetry reasons, we get the same for the Y point holonomy and its labels ν_{v_j}, while for the k-label we have to choose full $\mathbb{Z}$ itself. This leads us to the initially stated definition (7.22) with (7.24). However, this infinite linear combination of the basis states is a rather formal ansatz as its norm

$$\langle \varphi \,|\, \varphi \rangle = \|\varphi\|^2 = \sum_{k\in\mathbb{Z}^N} \sum_{\mu\in m} \sum_{\nu\in n} \sum_{k'\in\mathbb{Z}^N} \sum_{\mu'\in m} \sum_{\nu'\in n} (C_{k,\mu,\nu})^* \cdot C_{k',\mu',\nu'} \langle k,\mu,\nu | k',\mu',\nu' \rangle \tag{7.30}$$

$$= \sum_{k\in\mathbb{Z}^N} \sum_{\mu\in m} \sum_{\nu\in n} |C_{k,\mu,\nu}|^2 \tag{7.31}$$

diverges. We will need these extensive states for the beginning, but when it comes to zero volume eigenstates, e.g., we will also find states with finite norm (cf. Subsec. 7.2.1).

7.1.3 Action of the physical Hamiltonian $\hat{\mathrm{H}}_{\mathrm{phys}}$ on the ansatz states

We will now state the action of $\hat{\mathrm{H}}_{\mathrm{phys}}$ on the state $|\varphi\rangle$ given in (7.22). As the final result (7.39) will be rather long, we start with presenting the actions of $\hat{\mathrm{H}}_{\mathrm{eucl}}$ and $(\hat{\mathrm{H}}_{\mathrm{eucl}})^\dagger$ as well.

This is furthermore convenient since we will later also use them individually. According to the action of the operators on the basis states as listed in Subsection 7.1.1, we obtain

$$
\begin{aligned}
&\hat{\mathrm{H}}_{\mathrm{eucl}}\,|\varphi\rangle = \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}\,\hat{\mathrm{H}}_{\mathrm{eucl},v}\,\big|k,\mu,\nu\big\rangle \\
&= \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n}\kappa_{\mathrm{eucl}}C_{k,\mu,\nu}\Big\{\Big(\sqrt{\big|k_{e_v}+k_{e_{v^-}}+1\big|}-\sqrt{\big|k_{e_v}+k_{e_{v^-}}-1\big|}\Big)\sqrt{|\mu_v||\nu_v|}\cdot \\
&\quad\cdot\Big[\big|k,\mu_v+2,\nu_v+2\big\rangle-\big|k,\mu_v+2,\nu_v-2\big\rangle-\big|k,\mu_v-2,\nu_v+2\big\rangle+\big|k,\mu_v-2,\nu_v-2\big\rangle\Big]+ \\
&\quad+\sqrt{\big|k_{e_v}+k_{e_{v^-}}\big||\nu_v|}\Big(\sqrt{|\mu_v+1|}-\sqrt{|\mu_v-1|}\Big)\cdot \\
&\quad\cdot\Big[\big|k_{e_v}+2,\mu,\nu_v+1,\nu_{v^+}+1\big\rangle-\big|k_{e_v}+2,\mu,\nu_v+1,\nu_{v^+}-1\big\rangle+ \\
&\qquad+\big|k_{e_v}+2,\mu,\nu_v-1,\nu_{v^+}+1\big\rangle-\big|k_{e_v}+2,\mu,\nu_v-1,\nu_{v^+}-1\big\rangle- \\
&\qquad-\big|k_{e_v}-2,\mu,\nu_v+1,\nu_{v^+}+1\big\rangle+\big|k_{e_v}-2,\mu,\nu_v+1,\nu_{v^+}-1\big\rangle- \\
&\qquad-\big|k_{e_v}-2,\mu,\nu_v-1,\nu_{v^+}+1\big\rangle+\big|k_{e_v}-2,\mu,\nu_v-1,\nu_{v^+}-1\big\rangle\Big]+ \\
&\quad+\sqrt{\big|k_{e_v}+k_{e_{v^-}}\big||\mu_v|}\Big(\sqrt{|\nu_v+1|}-\sqrt{|\nu_v-1|}\Big)\cdot \\
&\quad\cdot\Big[\big|k_{e_v}+2,\mu_v+1,\mu_{v^+}+1,\nu\big\rangle-\big|k_{e_v}+2,\mu_v+1,\mu_{v^+}-1,\nu\big\rangle+ \\
&\qquad+\big|k_{e_v}+2,\mu_v-1,\mu_{v^+}+1,\nu\big\rangle-\big|k_{e_v}+2,\mu_v-1,\mu_{v^+}-1,\nu\big\rangle- \\
&\qquad-\big|k_{e_v}-2,\mu_v+1,\mu_{v^+}+1,\nu\big\rangle+\big|k_{e_v}-2,\mu_v+1,\mu_{v^+}-1,\nu\big\rangle- \\
&\qquad-\big|k_{e_v}-2,\mu_v-1,\mu_{v^+}+1,\nu\big\rangle+\big|k_{e_v}-2,\mu_v-1,\mu_{v^+}-1,\nu\big\rangle\Big]\Big\}
\end{aligned}
\tag{7.32}
$$

and likewise

$$
\begin{aligned}
&(\hat{\mathrm{H}}_{\mathrm{eucl}})^\dagger|\varphi\rangle = \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}(\hat{\mathrm{H}}_{\mathrm{eucl},v})^\dagger\big|k,\mu,\nu\big\rangle \\
&= \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n}\kappa_{\mathrm{eucl}}C_{k,\mu,\nu}\Big\{\Big(\sqrt{\big|k_{e_v}+k_{e_{v^-}}+1\big|}-\sqrt{\big|k_{e_v}+k_{e_{v^-}}-1\big|}\Big)\cdot \\
&\quad\cdot\Big[\sqrt{|\mu_v+2||\nu_v+2|}\big|k,\mu_v+2,\nu_v+2\big\rangle-\sqrt{|\mu_v+2||\nu_v-2|}\big|k,\mu_v+2,\nu_v-2\big\rangle- \\
&\qquad-\sqrt{|\mu_v-2||\nu_v+2|}\big|k,\mu_v-2,\nu_v+2\big\rangle+\sqrt{|\mu_v-2||\nu_v-2|}\big|k,\mu_v-2,\nu_v-2\big\rangle\Big]+ \\
&\quad+\Big(\sqrt{|\mu_v+1|}-\sqrt{|\mu_v-1|}\Big)\Big[\sqrt{\big|k_{e_v}+k_{e_{v^-}}+2\big||\nu_v+1|}\big|k_{e_v}+2,\mu,\nu_v+1,\nu_{v^+}+1\big\rangle- \\
&\qquad\qquad-\sqrt{\big|k_{e_v}+k_{e_{v^-}}+2\big||\nu_v+1|}\big|k_{e_v}+2,\mu,\nu_v+1,\nu_{v^+}-1\big\rangle+
\end{aligned}
$$

$$
\begin{aligned}
&+\sqrt{\left|k_{e_v}+k_{e_{v^-}}+2\right|\left|\nu_v-1\right|}\left|k_{e_v}+2,\mu,\nu_v-1,\nu_{v^+}+1\right\rangle-\\
&-\sqrt{\left|k_{e_v}+k_{e_{v^-}}+2\right|\left|\nu_v-1\right|}\left|k_{e_v}+2,\mu,\nu_v-1,\nu_{v^+}-1\right\rangle-\\
&-\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right|\left|\nu_v+1\right|}\left|k_{e_v}-2,\mu,\nu_v+1,\nu_{v^+}+1\right\rangle+\\
&+\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right|\left|\nu_v+1\right|}\left|k_{e_v}-2,\mu,\nu_v+1,\nu_{v^+}-1\right\rangle-\\
&-\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right|\left|\nu_v+1\right|}\left|k_{e_v}-2,\mu,\nu_v-1,\nu_{v^+}+1\right\rangle+\\
&+\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right|\left|\nu_v+1\right|}\left|k_{e_v}-2,\mu,\nu_v-1,\nu_{v^+}-1\right\rangle\Big]+\\
+\Big(\sqrt{|\nu_v+1|}-\sqrt{|\nu_v-1|}\Big)\Big[&\sqrt{\left|k_{e_v}+k_{e_{v^-}}+2\right|\left|\mu_v+1\right|}\left|k_{e_v}+2,\mu_v+1,\mu_{v^+}+1,\nu\right\rangle-\\
&-\sqrt{\left|k_{e_v}+k_{e_{v^-}}+2\right|\left|\mu_v+1\right|}\left|k_{e_v}+2,\mu_v+1,\mu_{v^+}-1,\nu\right\rangle+\\
&+\sqrt{\left|k_{e_v}+k_{e_{v^-}}+2\right|\left|\mu_v-1\right|}\left|k_{e_v}+2,\mu_v-1,\mu_{v^+}+1,\nu\right\rangle-\\
&-\sqrt{\left|k_{e_v}+k_{e_{v^-}}+2\right|\left|\mu_v-1\right|}\left|k_{e_v}+2,\mu_v-1,\mu_{v^+}-1,\nu\right\rangle-\\
&-\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right|\left|\mu_v+1\right|}\left|k_{e_v}-2,\mu_v+1,\mu_{v^+}+1,\nu\right\rangle+\\
&+\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right|\left|\mu_v+1\right|}\left|k_{e_v}-2,\mu_v+1,\mu_{v^+}-1,\nu\right\rangle-\\
&-\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right|\left|\mu_v+1\right|}\left|k_{e_v}-2,\mu_v-1,\mu_{v^+}+1,\nu\right\rangle+\\
&+\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right|\left|\mu_v+1\right|}\left|k_{e_v}-2,\mu_v-1,\mu_{v^+}-1,\nu\right\rangle\Big]\Big\}
\end{aligned}
\tag{7.33}
$$

Therein, we defined

$$
\kappa_{\mathrm{eucl}} := \frac{\ell_{\mathrm{P}}}{8\kappa' {\beta_{\mathrm{BI}}}^{3/2} k_0 \mu_0 \nu_0}. \tag{7.34}
$$

Note that we always collected the generated states in squared brackets [...] to provide some clarity within the long formulae. Also, we could have structured the formula above differently and especially combined terms with the same charge-dependent prefactors — like every pair within the series of eight states in (7.33). We refrained from doing so as the structure, as it is, offers an easier overview of the created recharged states. Lastly, we want to point out the first collection of newly created states in (7.33) that all have prefactors $\sim \sqrt{|\mu_v \pm 2||\nu_v \pm 2|}$. These are precisely the states that do not vanish if acting on trivially charged vertices and thus forced us to redefine the basis states by setting $k_{e_v} = -k_{e_{v^-}}$

for those in order to have their mutual prefactor $\sqrt{\left|k_{e_v}+k_{e_{v^-}}+1\right|}-\sqrt{\left|k_{e_v}+k_{e_{v^-}}-1\right|}$ vanish (confer Figure 7.1 and Figure 7.2 and their discussions). The corresponding actions of $\hat{\mathrm{H}}^{(1)}_{\mathrm{lor}}$ and $\hat{\mathrm{H}}^{(2)}_{\mathrm{lor}}$ are more compact and read

$$
\begin{aligned}
\hat{\mathrm{H}}^{(1)}_{\mathrm{lor}}\,|\varphi\rangle &= \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}\,\hat{\mathrm{H}}^{(1)}_{\mathrm{lor},v}\,\big|k,\mu,\nu\big\rangle \\
&= \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n}\kappa_{\mathrm{lor},1}C_{k,\mu,\nu}\Big\{-\big(k_{e_{v^+}}-k_{e_{v^-}}\big)^2\Big[\big|k_{e_v}+k_{e_{v^-}}\big|^r|\mu_v|^r|\nu_v|^r\cdot \\
&\quad\cdot\Big(\big|k_{e_v}+k_{e_{v^-}}+1\big|^{\frac{r}{2}}-\big|k_{e_v}+k_{e_{v^-}}-1\big|^{\frac{r}{2}}\Big)\Big(|\mu_v+1|^{\frac{r}{2}}-|\mu_v-1|^{\frac{r}{2}}\Big)\cdot \\
&\quad\cdot\Big(|\nu_v+1|^{\frac{r}{2}}-|\nu_v-1|^{\frac{r}{2}}\Big)\Big]^l\Big\}\Big|_{r=\frac{2}{3}-\frac{1}{3l}}\big|k,\mu,\nu\big\rangle
\end{aligned}
\tag{7.35}
$$

and

$$
\begin{aligned}
\hat{\mathrm{H}}^{(2)}_{\mathrm{lor}}\,|\varphi\rangle &= \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}\,\hat{\mathrm{H}}^{(2)}_{\mathrm{lor},v}\,\big|k,\mu,\nu\big\rangle \\
= \sum_{v\in V(\alpha)}&\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n}\kappa_{\mathrm{lor},2}C_{k,\mu,\nu}\Big\{\big(k_{e_v}+k_{e_{v^-}}\big)^4(\mu_v\nu_{v^+}-\mu_{v^+}\nu_v)^2\Big[\big|k_{e_v}+k_{e_{v^-}}\big|^{r_2}|\mu_v|^{r_2}\cdot \\
&\cdot|\nu_v|^{r_2}\Big(\big|k_{e_v}+k_{e_{v^-}}+1\big|^{\frac{r_2}{2}}-\big|k_{e_v}+k_{e_{v^-}}-1\big|^{\frac{r_2}{2}}\Big)\Big(|\mu_v+1|^{\frac{r_2}{2}}-|\mu_v-1|^{\frac{r_2}{2}}\Big)\cdot \\
&\cdot\Big(|\nu_v+1|^{\frac{r_2}{2}}-|\nu_v-1|^{\frac{r_2}{2}}\Big)\Big]^l\Big\}\Big|_{r_2=\frac{2}{3}-\frac{5}{3l}}\big|k,\mu,\nu\big\rangle,
\end{aligned}
\tag{7.36}
$$

where we collected all constants in

$$
\begin{aligned}
\kappa_{\mathrm{lor},1} &:= \frac{4\pi^2\ell_{\mathrm{P}}\sqrt{\beta_{\mathrm{BI}}}}{16\kappa'}\left(\frac{1}{2r^3k_0\mu_0\nu_0}\right)^l\Bigg|_{r=\frac{2}{3}-\frac{1}{3l}} \quad\text{and} \\
\kappa_{\mathrm{lor},2} &:= \frac{4\pi^2\ell_{\mathrm{P}}\sqrt{\beta_{\mathrm{BI}}}}{16\kappa'}\left(\frac{1}{2{r_2}^3k_0\mu_0\nu_0}\right)^l\Bigg|_{r_2=\frac{2}{3}-\frac{5}{3l}}.
\end{aligned}
\tag{7.37}
$$

We can now combine all these contributions to state the full action of $\hat{\mathrm{H}}_{\mathrm{phys}}$:

$$
\begin{aligned}
&\hat{\mathrm{H}}_{\mathrm{phys}}\,|\varphi\rangle = \\
&= \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}\Big\{\frac{1}{2}\,\hat{\mathrm{H}}_{\mathrm{eucl},v}+\frac{1}{2}(\hat{\mathrm{H}}_{\mathrm{eucl},v})^\dagger+\hat{\mathrm{H}}^{(1)}_{\mathrm{lor},v}+\hat{\mathrm{H}}^{(2)}_{\mathrm{lor},v}\Big\}\big|k,\mu,\nu\big\rangle
\end{aligned}
\tag{7.38}
$$

$$
\begin{aligned}
= \sum_{v\in V(\alpha)} \sum_{k\in\mathbb{Z}^N} \sum_{\mu\in m} \sum_{\nu\in n} C_{k,\mu,\nu} \Big\{ \frac{\kappa_{\text{eucl}}}{2} \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 1|} - \sqrt{|k_{e_v} + k_{e_{v^-}} - 1|} \Big) \cdot \\
\cdot \Big[\Big(\sqrt{|\mu_v + 2||\nu_v + 2|} + \sqrt{|\mu_v||\nu_v|} \Big) |k, \mu_v + 2, \nu_v + 2\rangle - \\
- \Big(\sqrt{|\mu_v + 2||\nu_v - 2|} + \sqrt{|\mu_v||\nu_v|} \Big) |k, \mu_v + 2, \nu_v - 2\rangle - \\
- \Big(\sqrt{|\mu_v - 2||\nu_v + 2|} + \sqrt{|\mu_v||\nu_v|} \Big) |k, \mu_v - 2, \nu_v + 2\rangle + \\
+ \Big(\sqrt{|\mu_- + 2||\nu_v - 2|} + \sqrt{|\mu_v||\nu_v|} \Big) |k, \mu_v - 2, \nu_v - 2\rangle |k, \mu_v - 2, \nu_v - 2\rangle \Big] + \\
+ \kappa_{\text{eucl}} \Big(\sqrt{|\mu_v + 1|} - \sqrt{|\mu_v - 1|} \Big) \cdot \\
\cdot \Big[\Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 2||\nu_v + 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\nu_v|} \Big) |k_{e_v} + 2, \mu, \nu_v + 1, \nu_{v^+} + 1\rangle - \\
- \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 2||\nu_v + 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\nu_v|} \Big) |k_{e_v} + 2, \mu, \nu_v + 1, \nu_{v^+} - 1\rangle + \\
+ \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 2||\nu_v - 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\nu_v|} \Big) |k_{e_v} + 2, \mu, \nu_v - 1, \nu_{v^+} + 1\rangle - \\
- \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 2||\nu_v - 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\nu_v|} \Big) |k_{e_v} + 2, \mu, \nu_v - 1, \nu_{v^+} - 1\rangle - \\
- \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} - 2||\nu_v + 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\nu_v|} \Big) |k_{e_v} - 2, \mu, \nu_v + 1, \nu_{v^+} + 1\rangle + \\
+ \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} - 2||\nu_v + 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\nu_v|} \Big) |k_{e_v} - 2, \mu, \nu_v + 1, \nu_{v^+} - 1\rangle - \\
- \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} - 2||\nu_v - 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\nu_v|} \Big) |k_{e_v} - 2, \mu, \nu_v - 1, \nu_{v^+} + 1\rangle + \\
+ \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} - 2||\nu_v - 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\nu_v|} \Big) |k_{e_v} - 2, \mu, \nu_v - 1, \nu_{v^+} - 1\rangle \Big] + \\
+ \kappa_{\text{eucl}} \Big(\sqrt{|\nu_v + 1|} - \sqrt{|\nu_v - 1|} \Big) \cdot \\
\cdot \Big[\Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 2||\mu_v + 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\mu_v|} \Big) |k_{e_v} + 2, \mu_v + 1, \mu_{v^+} + 1, \nu\rangle - \\
- \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 2||\mu_v + 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\mu_v|} \Big) |k_{e_v} + 2, \mu_v + 1, \mu_{v^+} - 1, \nu\rangle + \\
+ \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 2||\mu_v - 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\mu_v|} \Big) |k_{e_v} + 2, \mu_v - 1, \mu_{v^+} + 1, \nu\rangle - \\
- \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} + 2||\mu_v - 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\mu_v|} \Big) |k_{e_v} + 2, \mu_v - 1, \mu_{v^+} - 1, \nu\rangle - \\
- \Big(\sqrt{|k_{e_v} + k_{e_{v^-}} - 2||\mu_v + 1|} + \sqrt{|k_{e_v} + k_{e_{v^-}}||\mu_v|} \Big) |k_{e_v} - 2, \mu_v + 1, \mu_{v^+} + 1, \nu\rangle +
\end{aligned}
$$

$$
\begin{aligned}
&+\left(\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right||\mu_v+1|}+\sqrt{\left|k_{e_v}+k_{e_{v^-}}\right||\mu_v|}\right)|k_{e_v}-2,\mu_v+1,\mu_{v^+}-1,\nu\rangle-\\
&-\left(\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right||\mu_v-1|}+\sqrt{\left|k_{e_v}+k_{e_{v^-}}\right||\mu_v|}\right)|k_{e_v}-2,\mu_v-1,\mu_{v^+}+1,\nu\rangle+\\
&+\left(\sqrt{\left|k_{e_v}+k_{e_{v^-}}-2\right||\mu_v-1|}+\sqrt{\left|k_{e_v}+k_{e_{v^-}}\right||\mu_v|}\right)|k_{e_v}-2,\mu_v-1,\mu_{v^+}-1,\nu\rangle\Bigg]-\\
&-\kappa_{\mathrm{lor},1}\left(k_{e_{v^+}}-k_{e_{v^-}}\right)^2\Big[\left|k_{e_v}+k_{e_{v^-}}\right|^r|\mu_v|^r|\nu_v|^r\left(\left|k_{e_v}+k_{e_{v^-}}+1\right|^{\frac{r}{2}}-\left|k_{e_v}+k_{e_{v^-}}-1\right|^{\frac{r}{2}}\right)\cdot\\
&\cdot\left(|\mu_v+1|^{\frac{r}{2}}-|\mu_v-1|^{\frac{r}{2}}\right)\left(|\nu_v+1|^{\frac{r}{2}}-|\nu_v-1|^{\frac{r}{2}}\right)\Big]^l|k,\mu,\nu\rangle+\\
&+\kappa_{\mathrm{lor},2}\left(k_{e_v}+k_{e_{v^-}}\right)^4(\mu_v\nu_{v^+}-\mu_{v^+}\nu_v)^2\Big[\left|k_{e_v}+k_{e_{v^-}}\right|^{r_2}|\mu_v|^{r_2}|\nu_v|^{r_2}\\
&\cdot\left(\left|k_{e_v}+k_{e_{v^-}}+1\right|^{\frac{r_2}{2}}-\left|k_{e_v}+k_{e_{v^-}}-1\right|^{\frac{r_2}{2}}\right)\left(|\mu_v+1|^{\frac{r_2}{2}}-|\mu_v-1|^{\frac{r_2}{2}}\right)\cdot\\
&\cdot\left(|\nu_v+1|^{\frac{r_2}{2}}-|\nu_v-1|^{\frac{r_2}{2}}\right)\Big]^l|k,\mu,\nu\rangle\Bigg\}\Bigg|_{r=\frac{2}{3}-\frac{1}{3l}\,\wedge\,r_2=\frac{2}{3}-\frac{5}{3l}}
\end{aligned}
\tag{7.39}
$$

Note that some contributions from $\hat{\mathrm{H}}_{\mathrm{eucl}}$ and $(\hat{\mathrm{H}}_{\mathrm{eucl}})^\dagger$ were combined, while some identical numerical charge-dependent prefactors were not factored out in order to keep a form that allows for an easy read-out of the newly created states.

7.2 On specific solutions of the Schrödinger-like equation

Having found an appropriate physical Hamiltonian (7.9) and states (7.21), we can approach solving the Schrödinger-like equation

$$
\mathrm{i}\hbar\,\partial_\tau|\Psi(\tau)\rangle=\hat{\mathrm{H}}_{\mathrm{phys}}\,|\Psi(\tau)\rangle. \tag{7.40}
$$

We already introduced the well-known separation ansatz

$$
|\Psi(\tau)\rangle=|\varphi(k,\mu,\nu)\rangle|\chi(\tau)\rangle \tag{7.21}
$$

for the states and we will later see that additional ansätze of this kind allow us to better understand the action of the physical Hamiltonian.

With this partitioning of the state, we can proceed to the time-independent version of the Schrödinger-like equation just like in standard quantum mechanics and obtain

$$\hat{\mathrm{H}}_{\mathrm{phys}}\,|\varphi\rangle = E|\varphi\rangle, \tag{7.41}$$

where we used E as the constant that arises due to the separation of the variables. This eigenvalue equation is now easier to solve, yet the involved action of the physical Hamiltonian makes it still very complicated to find general solutions. For this reason, we will first search for zero-volume eigenstates in the next subsection, as all terms of $\hat{\mathrm{H}}_{\mathrm{phys}}$ do indeed contain the volume operator this corresponds to the case $E = 0$. This is also an illustrative introduction in how to handle the action of operators on Gowdy states because determining the spectrum of $\hat{\mathrm{H}}_{\mathrm{phys}}$ is beyond the scope of this part. Furthermore, the special case of choosing $E = 0$ corresponds at the classical level to the limiting case where the dust energy density vanishes and thus should in some formal sense make contact to the vacuum Gowdy case. A more rigorous understanding of taking this limit in the quantum theory will be necessary in future work as well as analysing the question whether zero is involved in the spectrum of $\hat{\mathrm{H}}_{\mathrm{phys}}$ at all; both questions will not be addressed in this work. Here, considering this specific choice should rather be understood as an illustrative example in which we can obtain some first intuition about the action of the physical Hamiltonian operator on Gowdy states.

7.2.1 Zero-volume eigenstates

This subsection is about finding states $|\varphi\rangle$ for which the volume vanishes. While this certainly holds for trivially charged states $k_{e_v} = \mu_v = \nu_v = 0, \forall v \in V(\alpha)$, there are also ones with less rigid restrictions. We will use this subsection about finding those zero-volume states also as an introduction for what comes afterwards, as the technique of finding constraints for the coefficients $C_{k,\mu,\nu}$ such that the corresponding state $|\varphi\rangle$ features a desired property is the basis of our treatment of the Schrödinger-like equation, too.

We can derive the action of the volume operator on the states $|\varphi\rangle$ from (6.10):

$$\begin{aligned}\hat{\mathrm{V}}\,|\varphi\rangle &= \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}\,\hat{\mathrm{V}}_v\,\big|k,\mu,\nu\big\rangle \\ &= \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}\frac{1}{\sqrt{2}}\left(\frac{\beta_{\mathrm{BI}}\ell_{\mathrm{P}}{}^2}{2}\right)^{\frac{3}{2}}\sqrt{\big|k_{e_v}+k_{e_{v-}}\big|\,|\mu_v|\,|\nu_v|}\,\big|k,\mu,\nu\big\rangle.\end{aligned} \tag{7.42}$$

If we now want to find solutions for which the above eigenvalue vanishes, we deduce the condition

$$\sqrt{\left|k_{e_v} + k_{e_{v^-}}\right| |\mu_v| |\nu_v|} = 0 \; \forall v \in V(\alpha). \tag{7.43}$$

Note that contributions from different vertices can not sum up to zero as there are no negative eigenvalues, i.e. no negative volume contribution. This leads to the following basic conditions:

1. $k_{e_v} = 0 = k_{e_{v^-}}$ and μ_v, ν_v arbitrary
2. $k_{e_v} = -k_{e_{v^-}}$ and μ_v, ν_v arbitrary
3. $\mu_v = 0$ and k_{e_v}, ν_v arbitrary
4. $\nu_v = 0$ and k_{e_v}, μ_v arbitrary

The charges k_{e_v} play a special role as neighbouring k_{e_v} are coupled via $\sqrt{\left|k_{e_v} + k_{e_{v^-}}\right|}$. This is the reason why setting $k_{e_v} = 0$ is not sufficient for fulfilling (7.43), but instead at least $k_{e_{v^-}} = 0$ has to be chosen, too. Now, for having the total volume of $|\varphi\rangle$ to vanish, one may combine vertex-wise any of the above conditions. However, if one wants to construct zero-volume states, one rather works with the coefficients $C_{k,\mu,\nu}$. The above conditions for the charges then translate into conditions for the coefficients by assigning only to all those $C_{k,\mu,\nu}$ a non-zero value such that the thereby non-suppressed states $\left|k, \mu, \nu\right\rangle$ fulfil, as a set, for all vertices at least one of the above conditions. As an example, if we wish to have a state that has zero volume through $\mu_v = 0 \; \forall v \in V(\alpha)$, we set all those $C_{k,\mu,\nu}$ to zero whose set μ contains at least one $\mu_v \neq 0$:

$$\mu_v = 0 \; \forall v \in V(\alpha) \Longleftrightarrow C_{k,\mu,\nu} = 0 \text{ if } \exists v \in V(\alpha) \colon 0 \neq \mu_v \in \mu. \tag{7.44}$$

This way, by assigning specific values to certain coefficients $C_{k,\mu,\nu}$, we can construct states that fulfil a desired property such as having zero volume.

7.2.2 Vanishing action states for $\hat{\mathrm{H}}_{\mathrm{eucl}}$

The procedure of carrying over to conditions the coefficients $C_{k,\mu,\nu}$ have to satisfy can also be used to construct states that cause a vanishing action of $\hat{\mathrm{H}}_{\mathrm{eucl}}$. We exemplarily show this for the three-vertex graph — with basis states denoted by $|\varphi_3\rangle = \left|k, \mu, \nu\right\rangle_3$ — as it allows for clearer formulae. To keep our notation more compact, we use the abbreviations

$$v_I =: I, \tag{7.45}$$

$$\begin{aligned} k_{e_{v_I}} &=: k_I, & k_{e_{v_I^-}} &=: k_{I-1}, & k_{e_{v_I^+}} &=: k_{I+1}, \\ \mu_{v_I} &=: \mu_I, & \mu_{v^-} &=: \mu_{I-1}, & \mu_{v^+} &=: \mu_{I+1}, \\ \nu_{v_I} &=: \nu_I, & \nu_{v^-} &=: \nu_{I-1}, & \nu_{v^+} &=: \nu_{I+1}. \end{aligned} \tag{7.46}$$

With this notation, we deduce from (7.32) the following form of the action of $\hat{\mathrm{H}}_{\mathrm{eucl}}$ on $|\varphi_3\rangle$ after having performed substitutions of the charges so there is no shift in the basis states anymore:

$$\begin{aligned} &\hat{\mathrm{H}}_{\mathrm{eucl}} |\varphi_3\rangle = \sum_{I=1}^{3} \sum_{k\in\mathbb{Z}^3} \sum_{\mu\in m} \sum_{\nu\in n} C_{k,\mu,\nu}\, \hat{\mathrm{H}}_{\mathrm{eucl},v} \big|k,\mu,\nu\big\rangle_3 \\ &= \sum_{I=1}^{3} \sum_{k\in\mathbb{Z}^3} \sum_{\mu\in m} \sum_{\nu\in n} \kappa_{\mathrm{eucl}} \Bigg\{ \Big(\sqrt{|k_I + k_{I-1} + 1|} - \sqrt{|k_I + k_{I-1} - 1|} \Big) \cdot \\ &\quad \cdot \Big(C_{k,\mu_I-2,\nu_I-2} \sqrt{|\mu_I - 2||\nu_I - 2|} + C_{k,\mu_I+2,\nu_I+2} \sqrt{|\mu_I + 2||\nu_I + 2|} - \\ &\qquad - C_{k,\mu_I+2,\nu_I-2} \sqrt{|\mu_I + 2||\nu_I - 2|} - C_{k,\mu_I-2,\nu_I+2} \sqrt{|\mu_I - 2||\nu_I + 2|} \Big) + \\ &\quad + \Big(\sqrt{|\mu_I + 1|} - \sqrt{|\mu_I - 1|} \Big) \cdot \\ &\quad \cdot \Big[\big(C_{k_I+2,\mu,\nu_I+1,\nu_{I+1}+1} - C_{k_I+2,\mu,\nu_I+1,\nu_{I+1}-1} \big) \sqrt{|k_I + k_{I-1} + 2||\nu_I + 1|} + \\ &\qquad + \big(C_{k_I+2,\mu,\nu_I-1,\nu_{I+1}+1} - C_{k_I+2,\mu,\nu_I-1,\nu_{I+1}-1} \big) \sqrt{|k_I + k_{I-1} + 2||\nu_I - 1|} + \\ &\qquad + \big(C_{k_I-2,\mu,\nu_I+1,\nu_{I+1}-1} - C_{k_I-2,\mu,\nu_I+1,\nu_{I+1}+1} \big) \sqrt{|k_I + k_{I-1} - 2||\nu_I + 1|} + \\ &\qquad + \big(C_{k_I-2,\mu,\nu_I-1,\nu_{I+1}-1} - C_{k_I-2,\mu,\nu_I-1,\nu_{I+1}+1} \big) \sqrt{|k_I + k_{I-1} - 2||\nu_I - 1|} \Big]_\sharp + \\ &\quad + \Big(\sqrt{|\nu_I + 1|} - \sqrt{|\nu_I - 1|} \Big) \cdot \Big[\ldots (\mu \longleftrightarrow \nu) \ldots \Big]_\sharp \Bigg\} \big|k,\mu,\nu\big\rangle_3 . \end{aligned} \tag{7.47}$$

Therein, ≫ $\big[\ldots (\mu \longleftrightarrow \nu) \ldots \big]_\sharp$ ≪ stands for the square bracket with subscript $\sharp$ of the four lines before just with the roles of μ and ν interchanged. The notation for the coefficients $C_{k,\mu,\nu}$ is similar to the one of the states that we already used: Only the charges that were de- or increased are specifically denoted. The above formula is, of course, only possible since we sum over all charges from $-\infty$ to ∞ and the substitution therefore does not change the solution space.

Noticing that there is no mixing of the three classes of charges k, μ and ν, we introduce the separation ansatz

$$C_{k,\mu,\nu} = C_k \cdot C_\mu \cdot C_\nu. \tag{7.48}$$

With this, the above action becomes

$$\begin{aligned}
\hat{\mathrm{H}}_{\mathrm{eucl}} \left|\varphi_3\right\rangle = \sum_{I=1}^{3} \sum_{k\in\mathbb{Z}^3} \sum_{\mu\in m} \sum_{\nu\in n} \kappa_{\mathrm{eucl}} \Bigg\{ & C_k \Big(\sqrt{|k_I + k_{I-1} + 1|} - \sqrt{|k_I + k_{I-1} - 1|} \Big) \cdot \\
& \cdot \Big(C_{\mu_I+2}\sqrt{|\mu_I + 2|} - C_{\mu_I-2}\sqrt{|\mu_I - 2|} \Big) \cdot \Big(C_{\nu_I+2}\sqrt{|\nu_I + 2|} - C_{\nu_I-2}\sqrt{|\nu_I - 2|} \Big) + \\
& + \Big(C_{k_I+2}\sqrt{|k_I + k_{I-1} + 2|} - C_{k_I-2}\sqrt{|k_I + k_{I-1} - 2|} \Big) \cdot \\
& \cdot \Bigg[C_\mu \Big(\sqrt{|\mu_I + 1|} - \sqrt{|\mu_I - 1|} \Big) \Big(\Big(C_{\nu\,{}^{+}_{+}1} - C_{\nu\,{}^{+}_{-}1} \Big) \sqrt{|\nu_I + 1|} + \Big(C_{\nu\,{}^{-}_{+}1} - C_{\nu\,{}^{-}_{-}1} \Big) \sqrt{|\nu_I - 1|} \Big) \\
& + \quad \text{——"——}_{(\mu\longleftrightarrow\nu)} \qquad \Bigg] \Bigg\} \big| k, \mu, \nu \big\rangle_3,
\end{aligned} \tag{7.49}$$

where the last line's » $\text{——"——}_{(\mu\longleftrightarrow\nu)}$ « denotes the ditto mark of the line before with the roles of μ and ν interchanged. As before, while C_k stands for the coefficient representing all unshifted k-charges, C_{k_I+2} means that all but k_I are unshifted and k_I is increased by two. We then introduced a new abbreviation for coefficients that feature shifts in the charges of both v_I and v_{I+1}: $C_{\nu\,{}^{+}_{+}1} := C_{\nu_I+1,\nu_{I+1}+1}$, $C_{\nu\,{}^{+}_{-}1} := C_{\nu_I+1,\nu_{I+1}-1}$, $C_{\nu\,{}^{-}_{+}1} := C_{\nu_I-1,\nu_{I+1}+1}$ and $C_{\nu\,{}^{-}_{-}1} := C_{\nu_I-1,\nu_{I+1}-1}$.

To get an intuition of the formula above, we may consider graphs for which the action vanishes. We can then state two basic principles to achieve this — or, in fact, any other degeneracy, too:

1. The sum over the vertices causes the individual contributions to cancel each other / equal the desired value, or
2. each individual contribution vanishes / amounts for the same contribution to the desired value.

While for the last one we can ignore the sum over the vertices and just need to find coefficients that make up for $^1/_{\sharp(\text{vertices})}$-th of the final result's value, the first one is more complicated and we may not find general solutions that reflect, e.g., the symmetries of the Gowdy models. For that reason, we concentrate on solutions that fulfil the chosen constraint vertex-wise.

If we want (7.49) to vanish, we first of all notice that we face a sum of two contributions within the curly brackets. As the two are products and sums/differences of square roots, we may conclude that it is unlikely for the two to annihilate, although that can be achieved for specific choices. Hence, we want both summands to vanish on their own, which can be fulfilled, e.g., by

1. $C_{\mu_I+2}\sqrt{|\mu_I+2|} = C_{\mu_I-2}\sqrt{|\mu_I-2|}$
2. $C_{k_I+2}\sqrt{|k_I+k_{I-1}+2|} = C_{k_I-2}\sqrt{|k_I+k_{I-1}-2|}$.

The first choice is, of course, equivalently replaceable by the corresponding condition with $\mu_I \mapsto \nu_I$ due to the multiplicative structure of the first summand within (7.49). Likewise, one could replace the above second condition with one that makes the second summand of (7.49) vanish via a zero contribution from the square brackets. Considering this bracket's additive structure, in turn, more than one such condition would be required. Therefore, the above conditions can be considered as the most basic ones. The chart in Figure 7.3 illustrates what this condition means in terms of the three k_I-charges, after having gone over to the equivalent form

$$C_{k_I+4} = \sqrt{\frac{|k_I+k_{I-1}|}{|k_I+k_{I-1}+4|}}C_k : \tag{7.50}$$

Starting with a specific value for C_{111}, we can determine the value of, say, C_{115} afterwards. This means that there are two paths leading to the new value of C_{155}: Either via $C_{111} \to C_{115} \to C_{155}$ or $C_{111} \to C_{151} \to C_{155}$. Doing so, we get contradictory results for the two paths (confer Figure 7.3). This is due to the condition depending also on k_{I-1}. During the path via C_{151}, this charge was increased by four before being evaluated, while it was increased only after being evaluated during the other path — which is also why there the prefactor $\sqrt{2/6}$ appears in both steps. Lastly, note that the trivial solution is of course not excluded and marks the only scenario where the above contradiction does not apply. Even though this condition turned out to be inapplicable, it showed the general strategy we pursue — and where one has to be cautious. Proceeding to the condition for μ (or ν), we first of all notice that there is no link between the respective charges of different vertices. Therefore, we may separate the coefficients once more into

$$C_\mu = c_{\mu_1} \cdot c_{\mu_2} \cdot c_{\mu_3} \text{ and} \tag{7.51}$$

$$C_\nu = c_{\nu_1} \cdot c_{\nu_2} \cdot c_{\nu_3}. \tag{7.52}$$

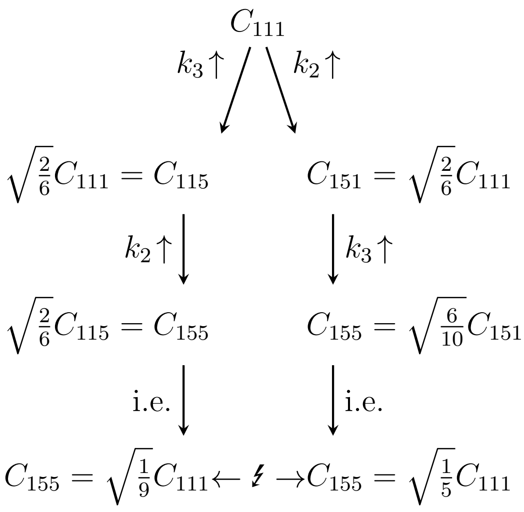


Figure 7.3: On the condition (7.50) on k

With this and moving the shift again into one of the coefficients only, the condition now reads

$$C_{\mu_I+2}\sqrt{|\mu_I+2|} = C_{\mu_I-2}\sqrt{|\mu_I-2|} \;\Rightarrow\; c_{\mu_I+4} = \sqrt{\frac{|\mu_I|}{|\mu_I+4|}}c_{\mu_I}. \tag{7.53}$$

This condition is, e.g., fulfilled by

$$c_{\mu_I} = \begin{cases} \text{arbitrary}, & \text{for } \mu_I = 0 \\ 0, & \forall \mu_I \in 4\mathbb{Z} \\ \sqrt{\frac{1}{|\mu_I|}}, & \text{rest} \end{cases} . \tag{7.54}$$

Due to the denominator diverging for $\mu_I = -4$, the first two cases of the solution above are rather formal. As the condition (7.53) is a recurrence relation of order 4, we chose the remaining three initial conditions as $c_1 = 1, c_2 = \sqrt{\frac{1}{2}}, c_3 = \sqrt{\frac{1}{3}}$ to obtain the intuitive solution (7.54). With this, we can now set the first part of the action to zero for all vertices. However, as shown before, we need a different procedure than the initially discussed one for the second part. Starting with the relevant part after the last separation, the square brackets of (7.49)

$$\begin{aligned}&\Big[\dots\Big]\big((7.49)\big) = \\ &= C_\mu\Big(\sqrt{|\mu_I+1|}-\sqrt{|\mu_I-1|}\Big)c_{\nu_{I+2}}\big(c_{\nu_{I+1}+1}-c_{\nu_{I+1}-1}\big)\Big(c_{\nu_I+1}\sqrt{|\nu_I+1|}+c_{\nu_I-1}\sqrt{|\nu_I-1|}\Big) \\ &\quad + \quad \text{——"——}_{(\mu\longleftrightarrow\nu)},\end{aligned} \tag{7.55}$$

we realise we can choose any of the following four options for making this expression vanish:

$$c_{\nu_{I+1}+1} - c_{\nu_{I+1}-1} = 0 \qquad \text{or} \tag{7.56a}$$
$$c_{\nu_I+1}\sqrt{|\nu_I+1|} + c_{\nu_I-1}\sqrt{|\nu_I-1|} = 0 \tag{7.56b}$$

and

$$c_{\mu_{I+1}+1} - c_{\mu_{I+1}-1} = 0 \qquad \text{or} \tag{7.57a}$$
$$c_{\mu_I+1}\sqrt{|\mu_I+1|} + c_{\mu_I-1}\sqrt{|\mu_I-1|} = 0. \tag{7.57b}$$

With the second line representing conditions on the c_{μ_I}, we have to guarantee compatibility with the previously obtained solution (7.54), or rather the constraint (7.53) behind it. However, it is easy to show that solutions of (7.57b) automatically fulfil (7.53):

$$(7.57\text{b}) \Rightarrow \begin{cases} c_{\mu_I+2}\sqrt{|\mu_I+2|} = -c_{\mu_I}\sqrt{|\mu_I|} \searrow \\ c_{\mu_I}\sqrt{|\mu_I|} = -c_{\mu_I-2}\sqrt{|\mu_I-2|} \nearrow \end{cases} \overset{\ominus}{\Rightarrow} c_{\mu_I+2}\sqrt{|\mu_I+2|} =$$
$$= c_{\mu_I-2}\sqrt{|\mu_I-2|} = (7.53). \tag{7.58}$$

Note that the inverse does not hold — solutions to (7.53) do not automatically also solve (7.57b). The proof thereof is analogous to (7.58).

In contrast to the condition (7.53) that we solved before, we now have its equivalent difference equation of second order and with alternating sign at hand. Hence, the solution to (7.57b) can be derived from (7.54):

$$c_{\mu_I}\Big|_{(7.57\text{b})} = \begin{cases} \text{arbitrary}, & \text{for } \mu_I = 0 \\ 0, & \forall \mu_I \in 2\mathbb{Z} \\ (-1)^{\frac{\mu_I-1}{2}}\sqrt{\frac{1}{|\mu_I|}}, & \text{rest} \end{cases}. \tag{7.59}$$

I.e., while it remains structurally the same, it considers the alternating minus sign and the necessity of setting every second coefficient zero — compared to every fourth one before.

With (7.59) and the adapted form for ν_I, we can achieve a vanishing action according to (7.49). Alternatively, we can replace one of the two by (7.57a) or (7.56a), whose solutions are obtained straightforwardly as

$$c_{\mu_I}\Big|_{(7.57a)} = \begin{cases} \text{arbitrary}, & \text{for } \mu_I \in \{0,1\} \\ c_0, & \forall \mu_I \in 2\mathbb{Z} \setminus \{0\} \\ c_1, & \forall \mu_I \in 2\mathbb{Z}+1 \setminus \{1\} \end{cases} \tag{7.60}$$

and the corresponding expression for ν_I. Note that (7.56a) and (7.57a) are conditions for vertices v_{I+1}, but as we sum over all vertices and try to find conditions that hold already vertex-wise, we can neglect that shift.

Summarising, we can make the action of $\hat{\mathrm{H}}_{\mathrm{eucl}}$ vanish by

$$(7.59)\Big|_{\mu_I} \wedge \Big((7.60)\Big|_{\nu} \vee (7.59)\Big|_{\nu}\Big) \tag{S1}$$

or, equivalently, with μ and ν interchanged. Note that these turn out to be the only two combinations of the solutions stated above: (7.55) showed that we need one condition for μ and one for ν as the solutions to (7.56a) and (7.56b) are not compatible (and likewise those to (7.57a) and (7.57b)). Furthermore, the solution (7.54) for either μ or ν, which makes the first part of the Euclidean action vanish, does not so for any contribution of the second part, (7.55). In turn, the condition (7.53) behind that solution is automatically fulfilled by solutions to (7.57b) (and, again, the same holds for the respective ν equivalents). Hence, we have to choose (7.59) for at least one of the charges μ and ν, which then makes one part of the Euclidean action's second contribution vanish as well as the first contribution. The remaining contribution then vanishes by setting (7.59) or (7.60) for the respective other set of charges.

We therefore found states $|\varphi\rangle := \sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}|k,\mu,\nu\rangle$ that experience a vanishing action of $\hat{\mathrm{H}}_{\mathrm{eucl}}$ by fulfilling constraints for the separated coefficients $C_{k,\mu,\nu} = C_k \prod_I c_{\mu_I} c_{\nu_I}$. The solution we stated above, however, poses restrictions for the μ and ν coefficients only.

7.2.3 Degeneracies of the action of the Lorentzian part $\hat{\mathrm{H}}_{\mathrm{lor}}$

While the diagonal action (7.61) of $\hat{\mathrm{H}}_{\mathrm{lor}}$ makes a discussion as the one of the previous subsection irrelevant — note that a diagonal action includes that there are no shifted coefficients —, it in turn allows for a discussion of degeneracies.

Recall the action of $\hat{\mathrm{H}}_{\mathrm{lor}}$ on the state $|\varphi\rangle$ via (7.35) and (7.36)

$$\begin{aligned}\hat{\mathrm{H}}_{\mathrm{lor}}\,|\varphi\rangle = \sum_{v\in V(\alpha)}\sum_{k\in\mathbb{Z}^N}\sum_{\mu\in m}\sum_{\nu\in n} C_{k,\mu,\nu}\Bigg\{\Bigg\{ &-\kappa_{\mathrm{lor},1}\big(k_{e_v}-k_{e_{v^-}}\big)^2\Big[\big|k_{e_v}+k_{e_{v^-}}\big|^r|\mu_v|^r|\nu_v|^r\cdot\\ &\cdot\Big(\big|k_{e_v}+k_{e_{v^-}}+1\big|^{\frac{r}{2}}-\big|k_{e_v}+k_{e_{v^-}}-1\big|^{\frac{r}{2}}\Big)\Big(|\mu_v+1|^{\frac{r}{2}}-|\mu_v-1|^{\frac{r}{2}}\Big)\cdot\\ &\cdot\ \Big(|\nu_v+1|^{\frac{r}{2}}-|\nu_v-1|^{\frac{r}{2}}\Big)\Big]^l\Bigg\}\Bigg|_{r=\frac{2}{3}-\frac{1}{3l}}+\\ +\Bigg\{\kappa_{\mathrm{lor},2}\big(k_{e_v}+k_{e_{v^-}}\big)^4&(\mu_v\nu_{v^+}-\mu_{v^+}\nu_v)^2\Big[\big|k_{e_v}+k_{e_{v^-}}\big|^{r_2}|\mu_v|^{r_2}\cdot\\ &\cdot|\nu_v|^{r_2}\Big(\big|k_{e_v}+k_{e_{v^-}}+1\big|^{\frac{r_2}{2}}-\big|k_{e_v}+k_{e_{v^-}}-1\big|^{\frac{r_2}{2}}\Big)\Big(|\mu_v+1|^{\frac{r_2}{2}}-|\mu_v-1|^{\frac{r_2}{2}}\Big)\cdot\\ &\cdot\Big(|\nu_v+1|^{\frac{r_2}{2}}-|\nu_v-1|^{\frac{r_2}{2}}\Big)\Big]^l\Bigg\}\Bigg|_{r_2=\frac{2}{3}-\frac{5}{3l}}\Bigg\}\big|k,\mu,\nu\big\rangle. \end{aligned} \tag{7.61}$$

We notice that i.a. due to the appearance of r and r_2 as different exponents in the two contributions (and in $\kappa_{\mathrm{lor},1}$ and $\kappa_{\mathrm{lor},2}$, confer (7.37)), it is very unlikely for the two contributions to result in the same value or annihilate each other. Therefore, we consider both summands alone.

From the vertex-wise composition follow immediately two of the most basic degeneracies, namely rotations and flips of the graph and its vertices. Rotations and their corresponding rearrangement of the vertices are described by

$$\forall v_I\in V(\alpha)\colon\, v_I\mapsto v_{I+n},\ \text{for some } n\in\mathbb{N}, \tag{S2}$$

while flips of a graph α with $N=|V(\alpha)|$ many vertices can be represented as

$$\forall v_I\in V(\alpha)\colon\, v_I\mapsto v_{N+1-I+n},\ \text{for some } n\in\mathbb{N}. \tag{S3}$$

With this, all charges μ_v and ν_v change their indices the same way. Hence, these two mappings do not change the value of (7.61) when the summation over all vertices is considered.

The other basic degeneracy is the interchange of all μ and ν charges,

$$\forall v\in V(\alpha)\colon\, \mu_v\mapsto\nu'_v\wedge\nu_v\mapsto\mu'_v. \tag{S4}$$

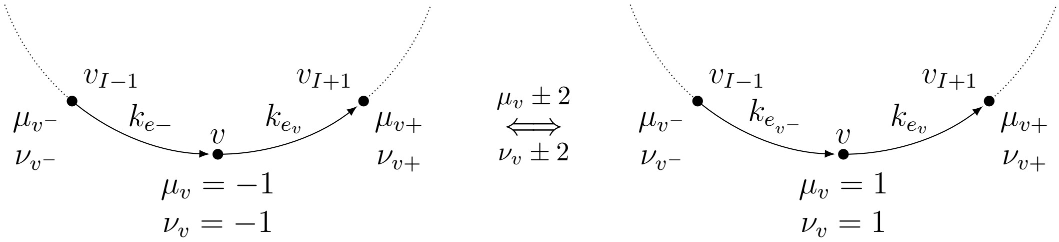
As for all considerations before, μ and ν play the same role in (7.61). The only factor that does not reflect this behaviour immediately is $(\mu_v \nu_{v^+} - \mu_{v^+}\nu_v)^2$, but due to the even exponent, the minus within the bracket that arises via the interchange of the μ and ν charges does not change its value as well.

After having specified these three basic degeneracies, an aspect of interest may be whether shifts created by the action of $\hat{\mathrm{H}}_{\mathrm{eucl}}$ result in a new degenerate state with the same eigenvalue of $\hat{\mathrm{H}}_{\mathrm{lor}}$. Addressing this question, we recapitulate that $\hat{\mathrm{H}}_{\mathrm{eucl}}$ acts only vertex-wise. Changing only the contribution of one vertex in (7.61), however, is in general not preserving its value, but we can indeed find configurations that do fulfil this connection of $\hat{\mathrm{H}}_{\mathrm{eucl}}$ and $\hat{\mathrm{H}}_{\mathrm{lor}}$. From (7.32), we recapitulate that $\hat{\mathrm{H}}_{\mathrm{eucl}} \big|k,\mu,\nu\big\rangle$ generates the shifted states

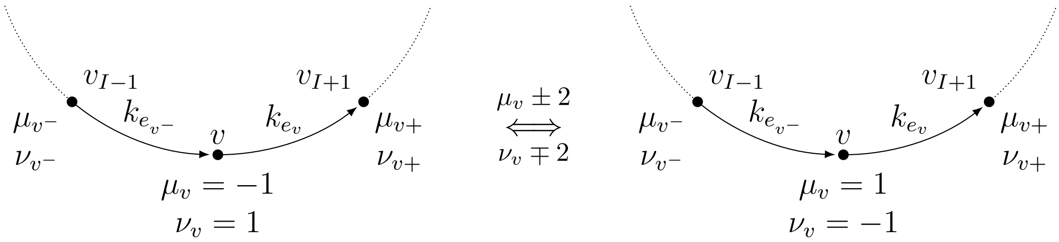
$$\big|k,\mu,\nu\big\rangle \overset{\hat{\mathrm{H}}_{\mathrm{eucl}}}{\mapsto} \big|k_{e_v} \pm 2, \mu_v \pm 1, \mu_{v^+} \pm 1, \nu\big\rangle, \big|k_{e_v} \pm 2, \mu, \nu_v \pm 1, \nu_{v^+} \pm 1\big\rangle, \big|k, \mu_v \pm 2, \nu_v \pm 2\big\rangle. \tag{7.62}$$

We then see that individual states of the set above do preserve some factors' values within (7.61) for specific values of the charges, but not the whole expression. It is in particular the link between the k-charges of different vertices that causes trouble: $\big(k_{e_v} + k_{e_{v^+}}\big)^4$ can not be preserved when only k_{e_v} is de- or increased by two. The only way that's possible is for $k_{e_v} = 0$ and $k_{e_v} = \pm 1$. But as we would have to fulfil it for every vertex, this choice leads to a contradiction. While this excludes the first two sets of states of (7.62), we can indeed find states of the third set that have the same Lorentz energy[2] as the initial $\big|k,\mu,\nu\big\rangle$. They are shown in Figure 7.4 and represent states where, at one vertex v, the charges μ_v and ν_v happen to be ± 1. Acting with $\hat{\mathrm{H}}_{\mathrm{eucl}}$ on such a state produces i.a. states of the third set of states of (7.62) that only change the signs of these charges μ_v and ν_v: from -1 to +1 or vice versa. This clearly preserves all factors $|\mu_v, \nu_v|^{r,r_2}$ of the Lorentz action (7.61) and also the products $\Big(|\mu_v + 1|^{\frac{r}{2},\frac{r_2}{2}} - |\mu_v - 1|^{\frac{r}{2},\frac{r_2}{2}}\Big)\Big(|\nu_v + 1|^{\frac{r}{2},\frac{r_2}{2}} - |\nu_v - 1|^{\frac{r}{2},\frac{r_2}{2}}\Big)$ due to the double change of the sign. Lastly, $(\mu_v \nu_{v^+} - \mu_{v^+}\nu_v)^2$ experiences a change of the sign in both its subtrahend and its minuend, hence preserves its value because of the square. Note that this factor has to be preserved for the vertex v_{I-1} as well, due to the mixture of the charges of the current and the next vertex. All other μ- and ν-charges as well as all k_{e_v} can, however, be chosen arbitrary as the symmetry of -1 and +1 suffices to conserve the Lorentz energy.

[2]We call the eigenvalues of $\hat{\mathrm{H}}_{\mathrm{lor}}$ "Lorentz energies", even though they are, of course, not necessarily one part/summand of the (proper) energy eigenvalues of $\hat{\mathrm{H}}_{\mathrm{phys}}$.



(a) parallel degeneracy



(b) cross degeneracy

Figure 7.4: Specific degeneracies of states linked by the action of $\hat{\mathrm{H}}_{\mathrm{eucl}}$. As before in the figures also here to keep the notation more compact we used $k_{e_{v_I}} \coloneqq k_I, \mu_{v_I} \coloneqq \mu_I$ and $\nu_{v_I} \coloneqq \nu_I$ etc.

To give a further example of a more special degeneracy, we deduce from (7.61) that the charges k_{e_v} always appear in the combination $k_{e_v} + k_{e_{v^+}}$ or $k_{e_{v^+}} - k_{e_{v^-}}$. This allows to set

$$k_{e_{v_I}} \mapsto \begin{cases} k_{e_{v_I}} \pm a & \text{for } I \in 2\mathbb{Z}, a \in \mathbb{R} \\ k_{e_{v_I}} \mp a & \text{for } I \in 2\mathbb{Z}+1, a \in \mathbb{R} \end{cases} \tag{S5}$$

for graphs with an even number of vertices and yet get the same Lorentz energy.

Chapter 8

Conclusion

In this part, we considered a reduced model with a polarised $\mathbb{T}^3$ Gowdy symmetry resulting from Gaussian dust coupled to general relativity and afterwards applying the symmetry reduction. The corresponding physical phase space has three independent canonical pairs consisting of Dirac observables associated with the connection and triad variables and describe an unconstrained U(1) gauge field theory. The evolution of these Dirac observables is generated by a physical Hamiltonian that itself is a Dirac observable. This classical model was taken as a starting point and quantised in the reduced LQG as well as the AQG framework in this work. In both cases, due to the symmetry of the classical physical Hamiltonian a graph-preserving quantisation was chosen in order to implement these symmetries also at the quantum level. The results presented here extend the ones in the literature in the following aspects: On the one hand, the models existing so far that use a loop but not hybrid quantisation [164, 195] have all applied a Dirac quantisation where a kinematical Hilbert space is chosen as an intermediate step on which the Hamiltonian, spatial diffeomorphism and Gauß constraints of the Gowdy model are implemented as operators. The physical Hilbert space then involves those physical states that are annihilated by all constraint operators. The model discussed in [165–167] considers a hybrid quantisation where the homogeneous modes are quantised using loop quantum gravity techniques whereas for the quantisation of the inhomogeneous modes a Fock quantisation has been chosen. They are thus not easy to relate to those models where no Fock quantisation has been used such as, e.g., full LQG. The model in [195] derives the full physical Hilbert space in a simpler setup where vacuum Gowdy spacetimes have been considered with an additional rotational symmetry. The model that comes most closely to the one discussed here is the one in [164] where similarities but also differences exist. The main difference is that [164] also follows a Dirac quantisation for the individual constraints with partly a different regularisation. Since also for their chosen regularisation the structure of the constraint operators is similarly complicated as the Schrödinger-like equation we obtain here, the physical Hilbert space of that model has not yet been derived. Furthermore, because one works with the Hamiltonian constraint instead of a physical Hamiltonian, the properties of the constraint algebra, as in the full theory, favour a graph-modifying quantisation of the Hamiltonian constraints. This yields a setup where the construction of semiclassical states as well as solutions of the constraint operator equations become more complicated compared to the model presented in this work due to the fact that operators modify the underlying graph they are acting on. In contrast, in the models presented here, the graph-preserving property comes in accordance with the requirement to implement classical symmetries also at the quantum level in the case of the reduced LQG model where the usual Ashtekar-Lewandowski representation is chosen for the physical Hilbert space. We further discussed the differences in the implementation of graph-preserving operators in the reduced LQG and AQG framework. Furthermore, because we couple Gaussian dust to gravity, the number of physical degrees of freedom differ in the two models. The one of [164] has just one independent degree of freedom, whereas here we have three. This is reflected in the fact that all geometric degrees of freedom encoded in the Dirac observables of the model presented here are unconstrained, while for the corresponding quantities on the kinematical Hilbert space described in [164] constraints still exist. We also derived the explicit form of the Schrödinger-like equation of the model in the AQG framework. This result provides an option for future work in which one can analyse this Schrödinger-like equation numerically or perform a semiclassical analysis of this equation in order to derive the corresponding effective model. As far as these future computations are considered, the model with polarised $\mathbb{T}^3$ Gowdy symmetry introduced here has — due to its symmetry reduction — the advantage that the volume operator acts diagonally on the basis states and hence the spectrum of the volume operator is known in the quantum theory. For semiclassical computations we therefore do not need to apply semiclassical perturbation theory along the lines of [60], as it is necessary for full LQG. As we do not analyse the Schrödinger-like equation in full detail here but just derive it for the model and then discuss some very specific zero volume solutions in order to obtain a first intuition on how the physical Hamiltonian operator acts, it will be an interesting question for future work to better understand whether the model in [164] can in some sense be embedded in the model presented here at the quantum level, when we extend our model by additional constraints that reduce the dust degrees of freedom and allow to go back to the vacuum case — and how this might be reflected in the solutions of the Schrödinger-like equation we obtain in this work.

Another scenario where we can get a notion of how the physical Hamiltonian and especially its Euclidean and Lorentzian parts (inter-)act is degenerate perturbation theory. First steps were already performed in [203], where the action of the symmetrised Euclidean part $\frac{1}{2}\left(\hat{\mathrm{H}}_{\mathrm{eucl}} + (\hat{\mathrm{H}}_{\mathrm{eucl}})^{\dagger}\right)$ is treated as a perturbation on top of the action of the Lorentzian part. However, as the complete set of degeneracies of $\hat{\mathrm{H}}_{\mathrm{lor}}$ is not known, a comprehensive treatment of that ansatz is not possible. The special cases considered in [203] still illustrate nicely the interplay of the actions of the two parts of the physical Hamiltonian and how one can in general approach degenerate perturbation theory for Gowdy models like the one considered herein.

Part III

Semiclassical matrix elements and singularity avoidance

Chapter 9

Motivation

Note that the content of this part, Part III, was already published in [2, 3].
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Part III of the work at hand is in particular about the question of singularity avoidance in loop quantum gravity and a new procedure for computing semiclassical expectation values in general. We start with introducing the loop quantum gravity setup in Chapter 10 and continue with Kummer's confluent hypergeometric functions in Chapter 11. They are the key part of the new mechanism that allows i.a. to compute semiclassical expectation values of operators like the momentum operator to the power of a rational number. At the beginning of Chapter 11, we present the basic properties of Kummer's functions that will be used throughout this part of the work at hand. As a warm up example, we discuss in Section 11.3 fractional powers of momentum operators in the standard quantum mechanical case and compute their semiclassical expectation values analytically by means of Kummer's functions and their Fourier transforms, respectively. We then also compute the semiclassical expectation value of an operator that mimics the operator of interest in the loop quantum gravity part. As a comparison with this result via Kummer's functions, we apply in Section 11.4 a different technique of computing fractional powers of operators in a more general context, called the AQG-III algorithm [60].

The applications of the new procedure are then two-fold: We first consider coherent states on the circle in Chapter 12 and then cover the realm of loop quantum gravity in the remainder of Part III.

9.1 Kummer's functions and coherent states on the circle

In Chapter 12, we discuss coherent states for a particle on a circle, which have for instance been discussed in earlier work in [204–208] and references therein. In [204–207], coherent states in the Hilbert space $L_2(S^1)$ were constructed by means of the so-called Zak transformation [209], whereas in [208] complexifier coherent states [133] for the group U(1) were used, leading finally to the same kind of coherent states. These complexifier coherent states have been introduced in the framework of loop quantum gravity for the group SU(2) and analyses of their properties can be found in [121, 134, 135], while we refer to [59, 60, 63–66] for further applications. Expectation values for elementary operators like (integer powers) of the holonomy as well as the momentum operator with respect to coherent states in $L_2(S^1)$, also called semiclassical expectation values, have been computed in [204–208]. These semiclassical expectation values can be understood as an expansion in a classicality parameter, denoted by t in our work. For the standard harmonic oscillator coherent states, this classicality parameter can be identified with $\hbar/(m\omega)$. One is then interested in the classical limit of the expectation values, that is when t is sent to zero. If a set of coherent states provides an appropriate description of the semiclassical sector of the given quantum theory, we expect that at least for the elementary operators the quantum theory is built from, the classical limit (zeroth order in the semiclassical parameter t) agrees with the corresponding classical theory. Such an analysis allows to check whether, for a given operator in the quantum theory, the considered coherent states are suitable. In [205–207], expectation values with respect to coherent states in $L_2(S^1)$ were expressed in terms of Jacobi's theta function and its derivatives, which naturally occurs once one applies the Zak transform onto a Gaussian — the theta function is the image of the Gaussian under the Zak transformation.

In the course of Chapter 12, we extend these former results in two directions. On the one hand, we generalise the computation of semiclassical expectation values from integers powers of momentum operators to fractional powers. The motivation for this comes from loop quantum gravity and loop quantum cosmology respectively where operators like the square root of the determinant of momentum operators play a pivotal role when the dynamics is quantised. This generalisation can be done by using Kummer's confluent hypergeometric functions of the first and second kind. A basic result [210] we will rely on is the fact that the Kummer functions of the first and second kind are mapped onto each other under Fourier transformations if their parameters are adjusted accordingly. This allows to compute those expectation values completely analytically without the need to use estimates or approximations for the integrals involved. In a further step, one can use the well-known asymptotic expansions of Kummer's functions in order to obtain an expansion in terms of $\hbar$ or any other classicality parameter. This also allows to compute the classical limit, the lowest order of that expansion, for this kind of expectation values.

The second direction we will explore is to consider the Zak transformation not only for obtaining coherent states in $L_2(S^1)$, as it has been done in [205–207], but also in the context of computing semiclassical expectation values. By using the basic properties of the Zak transformation, we can show that there exists a very simple relation between the semiclassical matrix elements in $L_2(\mathbb{R})$ and $L_2(S^1)$. For a given operator on $L_2(S^1)$ (or a suitable domain thereof), the semiclassical matrix elements can be understood as a Fourier series with Fourier coefficients made from the corresponding matrix elements in $L_2(\mathbb{R})$, which involve the counterpart of the operator on $L_2(\mathbb{R})$ as well as a translation operator. In particular, this means that any semiclassical matrix element in $L_2(S^1)$ is completely determined by these corresponding matrix elements in $L_2(\mathbb{R})$. Interestingly, the leading order term, that is the limit in which the semiclassical parameter vanishes, exactly agrees with the semiclassical result obtained in $L_2(\mathbb{R})$. The latter is just a consequence of the unitarity of the Zak transformation. This relation, obtained in Subsection 12.2.2, provides an alternative way for computing semiclassical matrix elements and expectation values, respectively. It might also allow to reconsider those techniques from a different angle that have been used in the context of U(1) complexifier coherent states in [63, 64, 134, 135, 208] in order to estimate semiclassical expectation values and to obtain the classical limit. Although we will restrict to the one-dimensional case here, the Zak transformation, and thus also the results presented here, can be easily generalised to higher finite dimensional systems. As a more complex application of these techniques, we will apply them to $U(1)^3$ coherent states, which are often used as a toy model for loop quantum gravity, in the follow-up chapters. There, we will be mainly interested in computing the semiclassical expectation values of dynamical operators as it has for instance been done in [63–66]. The usage of Kummer's functions in this context allows to analytically compute some parts that have been only estimated in earlier work.

This first part on applications of Kummer's confluent hypergeometric functions other than in quantum mechanics is structured as follows: Since, as in [208], we come from the complexifier coherent states, after a brief introduction to the Zak transformation, we apply it to the heat kernel. This is more convenient in this context, in contrast to using the harmonic oscillator coherent states directly. For this purpose, we use former work from [211] and as expected we end up with the same coherent states for $L_2(S^1)$. Given this set of coherent states, we compute semiclassical expectation values of operators involving fractional powers of the momentum operators in Subsection 12.2.1. The relation between semiclassical matrix elements in $L_2(\mathbb{R})$ and $L_2(S^1)$ is derived and discussed in Subsection 12.2.2. As an application of this relation, we recompute a couple of semiclassical matrix elements and expectation values respectively and show that we obtain the correct results. Section 12.3 briefly covers the connection between the Zak transformation and the Poisson resummation formula, which is an integral tool in the context of complexifier coherent states. Lastly, we discuss in Section 12.4 — based on results obtained in [212] — that the heat equation can be transformed into Kummer's differential equation for a specific choice of the parameters of Kummer's functions and thus Kummer's functions can be understood as solutions of the heat equation for certain choices of boundary data.

9.2 Kummer's functions in loop quantum gravity

Motivated by results in loop quantum cosmology (LQC) on the cosmological singularity avoidance, it is of big interest to find out whether singularities — and especially the Big Bang singularity — are resolved in the framework of full loop quantum gravity, too. Loop quantum cosmology is a quantum mechanical toy model of loop quantum gravity with a finite amount of degrees of freedom as it quantises general relativity not as a whole but only its symmetry reduced, cosmological sector. It was introduced by Bojowald in a series of papers [37–40] based on former work with Kastrup [213] and evolved quickly into an active field of research; see for instance [214–216] for reviews and the references therein. While the results of [41–45] are indeed very promising concerning the avoidance of the Big Bang singularity and replacing it by a big bounce accordingly, there is a lot of discussion on how LQC is embedded into full LQG [46–52]. Hence, it is of importance to also approach the possibility of singularity avoidance from the side of full LQG — guided by the seminal results of LQC where possible. In order to proceed into this direction, an analysis of the operators describing the quantum dynamics in LQG is necessary. One approach that addresses this question follows the strategy to obtain cosmological models from full LQG as for instance in [144, 217], where the latter relies on semiclassical techniques in order to obtain cosmological models from LQG. In general, the semiclassical sector of the theory provides a framework where this question is of interest. Entering this realm, in turn, requires that we have appropriate semiclassical states for the theory, which we can use for computing expectation values of the relevant operators such as for instance the inverse scale factor in this sector. For loop quantum gravity, SU(2) complexifier coherent states were constructed in [62], based on a complexification method introduced in [130, 218], which was later generalised to diffeomorphism invariant gauge theories [129]. In a series of papers [121, 133–135], it was shown that these complexifier coherent states fulfil the desired properties such as peakedness in the configuration, momentum and phase space representation or the Ehrenfest theorems, i.e. that they do reflect the behaviour of classical physics in zeroth order in $\hbar$, and that the commutator of two operators (divided by $\mathrm{i}\hbar$) resembles the Poisson bracket of the corresponding classical functions. Accordingly, those states are also referred to as semiclassical states and one can use them to perform a semiclassical analysis. One class of dynamical operators relevant in this context, denoted as $\hat{q}^j_e(r)$, constitutes the main ingredient of many quantum operators that are important for describing the theory's dynamics. As the inverse scale factor can be constructed from it as well, it is furthermore the main object of investigation when looking into singularity avoidance in cosmology. One of the reasons why this class of operators, however, is not easy to handle is that they contain the volume operator to the power of $r \in \mathbb{Q}$, making many analytical calculations impossible since the full spectrum of the volume operator is not known. This is the reason why we are forced to use estimates, approximations or simplified models if we want to proceed. As far as semiclassical investigations are concerned, so-called semiclassical perturbation theory was introduced in [60] that allows to replace the volume operator by a power series expansion in terms of operators that involve only integer powers of the flux operators. For those, semiclassical expectation values can be analytically computed if one uses the SU(2) complexifier coherent states as has been shown in [121, 133–135]. Another possibility is to replace the SU(2) coherent states by $\mathrm{U}(1)^3$ coherent states, which have the advantage that they diagonalise the volume operator.

In previous work [63, 64], Sahlmann and Thiemann presented i.a. a procedure for calculating expectation values with respect to $\mathrm{U}(1)^3$ complexifier coherent states of the operators that constitute the Hamiltonians of various fields being coupled to gravity, including the operator $\hat{q}_e^j(r)$. They were able to perform their calculations without the usage of estimates to solve the occurring integrals in the expectation value as they restricted their analysis to cubic graphs. However, their approach involves a Taylor expansion of quantities with fractional powers, which was crucial for obtaining analytical expressions as final results. Later, Brunnemann and Thiemann [65, 66] analysed the question of singularity avoidance in loop quantum gravity. In their work, they showed that the analogue of the inverse scale factor operator in LQG is unbounded from above on zero volume states. However, they found indeed an upper bound for the expectation value of the inverse scale factor operator with respect to $\mathrm{U}(1)^3$ coherent states at the Big Bang. In order to obtain this result, they applied a chain of estimates that allowed them to circumvent the evaluation of the initial integrals and instead replace them by ones that can be integrated analytically with the methods they used. The details will be discussed in Subsection 16.1.1. They conclude that singularity avoidance in LQG, if existing, has to be addressed differently than in LQC, but the existence of an upper bound of the inverse scale factor's expectation value with respect to coherent states at the Big Bang can be seen as a strong indication for the respective singularity's resolution at least in the semiclassical sector of the theory.

This part of the work at hand aims at revisiting the semiclassical analysis of the inverse scale factor operator by applying the new technique introduced before: Kummer's confluent hypergeometric functions can be used to analytically compute expectation values of fractional powers of the momentum operator with respect to $\mathrm{U}(1)$ coherent states or the well-known quantum mechanical coherent states. This technique also applies to $\mathrm{U}(1)^3$ coherent states frequently used in the earlier analysis of LQG. The reason why Kummer's functions fit well into this framework is that Kummer's functions of first and second kind are in some sense dual to each other under the Fourier transform, which was shown in [210] and heavily used and discussed in detail in [2]. The integrals at hand for the semiclassical expectation values result essentially in Kummer's confluent hypergeometric function of the first kind. If being interested in the semiclassical limit, one can subsequently make use of the asymptotic expansion for large arguments of Kummer's functions to obtain in zeroth order the result one would expect from the classical calculation. This expansion is performed in terms of the classicality parameter encoded in the coherent states, which is $\hbar$ in the case of the quantum mechanical coherent states. The aim of this part of the present work now is to apply this new procedure in the LQG-framework and calculate semiclassical expectation values there. An advantage of this method compared to the former analysis in [63–66] is that we are able to avoid estimates at certain stages of the computation since we can integrate fractional powers against Gaussians, whereas in the former work either Taylor expansions or estimates were necessary to substitute the involved fractional powers. In our analysis here, depending on the scenario we consider, we can perform our computations either even without the additional usage of estimates or with ones that are slightly better adapted to the fractional power of the operator. The scenarios we consider differ by the choice of the underlying graph, particularly its valence, or by the power of the operator $\hat{q}_e^j(r)$. We will show that we can on the one hand extend the method used by Sahlmann and Thiemann also to more general graphs than cubic ones and on the other hand adapt the procedure of Brunnemann and Thiemann with the use of Kummer's functions and compare their results to ours. The latter allows us further to discuss limitations and generalisations of existing estimates in this context.

These considerations are structured as follows: First, we use this new procedure to compute the expectation value of fractional powers of the momentum operator with respect to coherent states in Chapter 13 as an illustrating example.
In Chapter 14, we apply this method to the volume operator and perform semiclassical computations without the additional usage of estimates. Starting with graphs of cubic topology, we first calculate the basic building block of their semiclassical expectation value of $\hat{q}_{I_0}^{i_0}(r)$ with respect to $\mathrm{U}(1)^3$ coherent states in Section 14.2. We only illustrate the general procedure, which we summarise in a note on page 181, while the details of this calculation are moved to Appendix B. The final result can be found in (14.27) on page 183. Its specialisation to the case $p = 0$, which corresponds classically to the cosmological singularity, is shown in (14.31) on page 185. Afterwards, we discuss the semiclassical limit in Section 14.4, where the detailed derivation is presented in Appendix D.
In our next step in Chapter 15, we then proceed to higher valent vertices and, after a general introduction, apply the procedure of Sahlmann and Thiemann to these not necessarily cubic graphs in Section 15.1. The final result for the semiclassical expectation values of $\prod_{k=1}^{N} \hat{q}_{J_k}^{j_k}(r)$ via a generalised form of the procedure of Sahlmann and Thiemann can be found on page 198 in (15.20) and we close this chapter with a comparison of the two approaches in Section 15.2.
For more complicated and general scenarios, the relevant integrals cannot be solved by

the methods discussed in the former chapter and therefore, in Chapter 16, we discuss semiclassical computations for the volume operator that also rely on estimates. The first calculation of Subsection 16.1.1 follows the route of Brunnemann and Thiemann and — likewise to their result — also yields an upper bound for the inverse scale factor, but in our case is adopted in such a way that we use different estimates as we can then evaluate the integrals at hand by means of Kummer's functions. The semiclassical expectation values of $\hat{q}^{i_0}_{I_0}(r)$ using a generalised form of the estimates of Brunnemann and Thiemann is shown in (16.15) on page 208. The case $p = 0$ is separately discussed and can be found in (16.19) on page 209. A generalisation of the above procedure for $\prod_{k=1}^{N} \hat{q}^{j_k}_{J_k}(r)$ is given in (16.27) on page 211 and for the specific case $p = 0$ in (16.31) on page 212. The comparison of the way different estimates enter into the final result allows us to discuss the limitations of such estimates as well as finding new estimates that potentially improve the results, or at least let us understand the problems that arise due to the utilisation of them. These are illustrated in Section 16.2, which concludes in a comparison with the initial Brunnemann and Thiemann approach in Subsection 16.2.3. The final result for the semiclassical expectation values of $\hat{q}^{i_0}_{I_0}(r)$ using a new kind of estimate is presented in (16.41) on page 216 and in (16.42) on page 217 for the case $p = 0$. Considering a further new kind of estimate, the semiclassical expectation value of $\hat{q}^{i_0}_{I_0}(r)$ has been recalculated in (16.63) on page 222. Subsection 16.2.2 presents a brief overview over conditions we may impose on possible new estimates.

Chapter 10

The setup — $U(1)^3$, the operator $\hat{q}^{i_0}_{I_0}(r)$ and coherent states

Investigating these kind of questions, it is common practice [63–66] to replace the gauge group SU(2) by $U(1)^3$. While the qualitative meaning of the obtained results is not altered by this substitution [60, 134, 135], working with the Abelian $U(1)^3$ renders many calculations more palpable. This is why $U(1)^3$ is gladly used for approaching new problems or testing novel techniques.

Going over to $U(1)^3$ requires some changes, of course. However, the underlying graph γ will not be changed and we still collect all edges e in $E(\gamma)$ and all vertices v in $V(\gamma)$. Each of those edges e is now equipped with the Hilbert space $\mathcal{H}_e = L_2(U(1)^3, \mathrm{d}\mu_H)$, with the Haar measure $\mathrm{d}\mu_H$, and the holonomy flux algebra reads

$$\left[\hat{h}^j_e, \hat{p}^k_{e'}\right] = -\mathrm{i}\frac{{\ell_{\mathrm{P}}}^2}{a^2}\delta_{ee'}\delta^{jk}\hat{h}^k_{e'}, \quad \left[\hat{h}^j_e, \hat{h}^k_{e'}\right] = 0 \quad \text{and} \quad \left[\hat{p}^j_e, \hat{p}^k_{e'}\right] = 0. \tag{10.1}$$

Therein, a length scale a was introduced that allows us to work with dimensionless fluxes for later convenience. It originates from the construction of the coherent states and is used there to have at hand a dimensionless complexifier. Note that it also links the classicality parameter t with the Planck length ℓ_{P}: $t = {\ell_{\mathrm{P}}}^2/a^2$.

Concerning the basis states, the previously introduced spin network functions T_γ are replaced by so-called *charge network functions* T^{c}_γ for $U(1)^3$. The name derives from the fact that all edges e_I are now "charged" with three U(1)-charges $n^i_I, i \in \{1, 2, 3\}$. The holonomy operator $\hat{h}^i_I$ acts on these states via multiplication and increases the corresponding charge n^i_I of the U(1)-copy i of the edge e_I by 1. The flux operator then acts via differentiation: $\hat{p}^j_e = \frac{\mathrm{i}}{a^2} h^j_e \frac{\partial}{\partial h^j_e}$.

The main operator of interest, or rather class of operators, is the previously mentioned

$$\hat{q}^j_e(r) := \operatorname{tr}\left(\tau_j \hat{h}_e \left[\left(\hat{h}_e\right)^{-1}, \hat{\mathrm{V}}^r\right]\right). \tag{10.2}$$

Its components are a basis τ_j of $\mathfrak{su}(2)$, the holonomy operator $\hat{h}_e$ acting on edge e and the volume operator $\hat{\mathrm{V}}$ to the power of $r \in \mathbb{Q}$. We already stated the latter in Subsection 2.4.2 as

$$\hat{\mathrm{V}} = {\ell_{\mathrm{P}}}^3 \sum_{v \in V(R)} \sqrt{\left| \frac{1}{48} \sum_{e_I \cap e_J \cap e_K = v} \epsilon^{ijk} \epsilon(e_I, e_J, e_K) \hat{J}^{(v,e_I)}_i \hat{J}^{(v,e_J)}_j \hat{J}^{(v,e_K)}_k \right|} \tag{10.3}$$

$$= {\ell_{\mathrm{P}}}^3 \sum_{v \in V(R)} \sqrt{\left|\hat{\mathrm{Q}}_v\right|}. \tag{10.4}$$

The great importance of this class of operators in the framework of loop quantum gravity now stems from their appearance in various (matter) Hamiltonian operators [63, 64] via products of the form

$$\prod_{k=1}^{N} \hat{q}^{j_k}_{e_k}.$$

Yet, they also are indeed crucial when tackling the question of singularity avoidance as the inverse scale factor can be obtained by setting $r = \frac{1}{2}, N = 6$ and multiplying by an additional $1/{\ell_{\mathrm{P}}}^{12}$ in order to get the dimensions right.

The $U(1)^3$-equivalent we will work with reads

$$\hat{q}^{i_0}_{I_0}(r) := \frac{1}{a^{3r}} \hat{h}^{i_0}_{I_0} \left[\left(\hat{h}^{i_0}_{I_0}\right)^{-1}, \hat{V}^r\right], \tag{10.5}$$

where we again considered the length scale a in order to work with dimensionless quantities. We adopted from [66] the marker $_0$ to highlight the specific U(1)-copy and edge the holonomies act on. The benefit of this will become clear soon.

For the action of $\hat{q}^{i_0}_{I_0}(r)$ on charge network functions, we first state the action of the volume operator on a charge network state:

$$\hat{V}\, T^{\mathrm{c}}_\gamma =: \lambda\big(\{n^i_I\}\big) T^{\mathrm{c}}_\gamma = \sum_v {\ell_{\mathrm{P}}}^3 \sqrt{\left| Z \sum_{I,J,K} \epsilon_{ijk}\epsilon(IJK) n^i_I n^j_J n^k_K \right|}\, T^{\mathrm{c}}_\gamma, \tag{10.6}$$

where we chose $Z := \frac{\beta^3}{48}$ [89]. The notation is in accordance with the literature [66], in particularly with regard to naming the eigenvalues $\lambda(\{n^i_I\})$. Therein, $\{n^i_I\}$ highlights that λ depends on the whole set of the charges n^i_I. We see that the charge network functions diagonalise the volume operator — another key advantage of $\mathrm{U}(1)^3$. The structure of the eigenvalues, accordingly, follows closely that of the volume operator itself: First, the action is vertex-wise and we sum over all vertices $v \in V(\gamma)$. Then, the square root collects in its argument all combinations of configurations of three edges e_I, e_J, e_K that meet at v (note that we abbreviated $\sum_{e_I\cap e_J \cap e_K = v}$ by $\sum_{I,J,K}$), covering their respective orientation via $\epsilon(IJK)$. The quantity this sum collects is what we may call the determinant of the "charge matrix": $\epsilon_{ijk} n^i_I n^j_J n^k_K$, where one dimension of the matrix is spanned by the three edges e_I, e_J, e_K and the other one by the three copies of $\mathrm{U}(1)$, labelled by i, j, k.

With this, we can now state the action of $\hat{q}^{i_0}_{I_0}(r)$ on charge network states T^{c}_γ [66]:

$$\begin{aligned} a^{3r} \cdot \hat{q}^{i_0}_{I_0}(r) T^{\mathrm{c}}_\gamma &= \left(\hat{\mathrm{V}}^r - \hat{h}^{i_0}_{I_0} \hat{\mathrm{V}}^r \left(\hat{h}^{i_0}_{I_0}\right)^{-1} \right) T^{\mathrm{c}}_\gamma \\ &= \big(\lambda^r\big(\{n^i_I\}\big) - \lambda^r\big(\{n^i_I - \delta^{ii_0}\delta_{II_0}\}\big)\big) T^{\mathrm{c}}_\gamma. \end{aligned} \tag{10.7}$$

We see that the eigenvalue of the volume operator changes for the contribution in which the (inverse) holonomy acting on edge e_{I_0} and U(1)-copy i_0 is involved. The inverse holonomy decreases the charge $n^{i_0}_{I_0}$ by 1 and hence, the volume operator sees only this reduced value when acting on $\left(\hat{h}^{i_0}_{I_0}\right)^{-1} T^{\mathrm{c}}_\gamma$. The following non-inverse holonomy then reproduces T^{c}_γ and we obtain the above difference of the "normal" volume eigenvalue and one experiencing a shift.

Much of the obstacles we will be facing during the upcoming investigations stems from the involved structure of (10.6). Computing semiclassical expectation values means to integrate these eigenvalues against Gaussian functions, which is not per se possible. This means that one either has to turn towards simplified configurations, where one can indeed perform the integration(s). Or, alternatively, one pursues the approximative part and tries to deduce estimates that allow finding upper bounds for the expression of interest. Over the next sections, we will delve into both branches.

The last ingredient of our setup are the complexifier coherent states for U(1)^3. We already introduced them in Subsection 2.7, (2.164):

$$\Psi_m(A) = \prod_{\substack{e_I \in E(\gamma)\\ i=1,2,3}} \sum_{\{n^i_I\}\in\mathbb{Z}} \mathrm{e}^{-\frac{t}{2}\left(n^i_I\right)^2 + n^i_I p^i_I(m)} \left[\mathrm{e}^{\mathrm{i}\theta^i_I(m)} \mathrm{e}^{-\mathrm{i}\theta^i_I(A)}\right]^{n^i_I}. \tag{10.8}$$

As a brief recap, $m = \left(A^{(0)}(x), E^{(0)}(x)\right)$ is the point the coherent state is peaked around and the quantity t is called the classicality parameter as the limit $t \to 0$ reflects entering the classical realm of the theory. In one exponent, we find p^i_I — the canonical conjugate of the holonomy, entering via the complexified holonomy. The whole expression shows clearly the edge- and U(1)-copy-wise structure of the coherent states. What is more, the coherent state is built up by the inverse holonomy, as one can infer from the minus sign in the square bracket's term $\mathrm{e}^{-\mathrm{i}\theta^i_I(A)}$. Accordingly, the coherent states are in fact linear combinations of the conjugate charge network functions $\overline{T}^{\mathrm{c}}_\gamma$. With this minus sign, the action of an additional inverse holonomy $\left(\hat{h}^{i_0}_{I_0}\right)^{-1}$, as happening in the second part of the operator of interest $\hat{q}^{i_0}_{I_0}(r)$, will not decrease the corresponding charge n^i_I by 1 but instead increase it. Having this in mind, we can now state the expectation value of $\hat{q}^{i_0}_{I_0}(r)$ with respect to the coherent states:

$$\begin{aligned}
\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m} &= \frac{1}{\|\Psi_m\|^2 a^{3r}} \sum_{\{n^i_I\}\in\mathbb{Z}} \mathrm{e}^{\sum_{i,I}\left(-t\left(n^i_I\right)^2 + 2p^i_I n^i_I\right)} \lambda^r\left(\left\{n^{i_0}_{I_0}\right\}\right)\\
&:= \frac{1}{\|\Psi_m\|^2 a^{3r}} \sum_{\{n^i_I\}\in\mathbb{Z}} \mathrm{e}^{\sum_{i,I}\left(-t\left(n^i_I\right)^2 + 2p^i_I n^i_I\right)} \left(\lambda^r\left(\left\{n^i_I\right\}\right) - \lambda^r\left(\left\{n^i_I + \delta^{ii_0}_{II_0}\right\}\right)\right)\\
&= \frac{1}{\|\Psi_m\|^2 a^{3r}} \sum_{\{n^i_I\}\in\mathbb{Z}} \mathrm{e}^{\sum_{i,I}\left(-t\left(n^i_I\right)^2 + 2p^i_I n^i_I\right)} {\ell_{\mathrm{P}}}^{3r} |Z|^{\frac{r}{2}} \left(\left|\sum_{IJK} \epsilon(IJK)\epsilon_{ijk} n^i_I n^j_J n^k_K\right|^{\frac{r}{2}} -\right.\\
&\qquad \left. - \left|\sum_{IJK} \epsilon(IJK)\epsilon_{ijk}\left(n^i_I + \delta^{ii_0}\delta_{II_0}\right)\left(n^j_J + \delta^{ji_0}\delta_{JI_0}\right)\left(n^k_K + \delta^{ki_0}\delta_{KI_0}\right)\right|^{\frac{r}{2}}\right).
\end{aligned} \tag{10.9}$$

We first of all defined the eigenvalue as $\lambda^r\left(\left\{n^{i_0}_{I_0}\right\}\right)$, where the indices tell the specific charge the (inverse) holonomy acts on and we kept the curly brackets to indicate that it still depends on all the charges of the state. The last line now reflects the aforementioned fact that acting on the conjugate charge network functions, the inverse holonomy will act by adding 1 to the shifted charge $n^{i_0}_{I_0}$. We also introduced in the second line $\delta^{ii_0}_{II_0}$ as a shorthand notation for $\delta^{ii_0}\delta_{II_0}$.

When it comes to the computation of expressions like (10.9) in the light of a semiclassical analysis, sending the classicality parameter t towards zero causes calculatory difficulty: With t becoming smaller and smaller, the Gaussian functions with $t(n^i_I)^2$ as their argument become wider and wider — forcing us to consider more and more contributions of the sum over all charges. What one would instead prefer to have at hand is an expression that converges quickly for $t \to 0$. The typical tool to achieve this is the so-called *Poisson resummation formula* [65, 66, 121, 130, 133–135, 218] and, in fact, after applying it we will ultimately only have to consider one contribution, which is even the trivial one.

Poisson resummation formula [134, Theorem 4.1]: For functions $f \in L_1(\mathbb{R}, \mathrm{d}x)$ for which

$$F(x) \coloneqq \sum_{n=-\infty}^{\infty} f(x + nT) \ , T > 0, \tag{10.10}$$

is absolutely and uniformly convergent for $x \in [0, T]$, the (re-)summation formula

$$\sum_{n=-\infty}^{\infty} f(nT) = \frac{2\pi}{T} \sum_{N=-\infty}^{\infty} \tilde{f}\left(\frac{2\pi N}{T}\right) \tag{10.11}$$

with the Fourier transform $\tilde{f}(k) = \int\limits_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x)$ of $f(x)$ holds.

To apply the Poisson resummation formula close to literature [66] in matters of notation, we first define

$$T \coloneqq \sqrt{t} \tag{10.12}$$

$$x^i_I \coloneqq T n^i_I \tag{10.13}$$

and then get

$$\langle \hat{q}^{i_0}_{I_0}(r) \rangle_{\Psi_m} = \frac{|Z|^{\frac{r}{2}} T^{3r}}{\|\Psi_m\|^2} \sum_{\{N^i_I\} \in \mathbb{Z}} \left(\frac{2\pi}{T}\right)^{3M} \int\limits_{-\infty}^{\infty} \mathrm{d}^9 x^i_I \; \mathrm{e}^{\sum_{i,I}\left(-\left(x^i_I\right)^2 + 2\frac{p^i_I - \pi\mathrm{i}N^i_I}{T} x^i_I\right)} \frac{1}{T^{3r}}$$

$$\cdot\left(\left|\sum_{IJK}\epsilon(IJK)\epsilon_{ijk}x^i_I x^j_J x^k_K\right|^{\frac{r}{2}} - \right.$$
$$\left. -\left|\sum_{IJK}\epsilon(IJK)\epsilon_{ijk}\big(x^i_I + T\delta^{ii_0}\delta_{II_0}\big)\big(x^j_J + T\delta^{ji_0}\delta_{JI_0}\big)\big(x^k_K + T\delta^{ki_0}\delta_{KI_0}\big)\right|^{\frac{r}{2}}\right). \tag{10.14}$$

Now, there are remarks to be made. First, we used the fact that we can associate the classicality parameter t with the Planck length ℓ_{P} and the length scale a via $T = \sqrt{t} = \frac{\ell_{\mathrm{P}}}{a}$. Second, the new "pseudo-charges" N^i_I that enter our formulae via the Poisson resummation formula are, in fact, not linked in any way to the previous U(1)-charges n^i_I. So whenever we talk about values of N^i_I, this does not transfer to the same information about n^i_I. This will become especially important when we consider solutions $\{N^i_I\} = 0$ only.

Similarly to above and following again the notation of [66], applying the Poisson resummation formula to the norm of the coherent states results in

$$\|\Psi_m\|^2 = \prod_{\substack{e_I\in E(\gamma)\\ i\in 1,2,3}}\sum_{N^i_I\in\mathbb{Z}} 2\pi\sqrt{\frac{\pi}{t}}\,\mathrm{e}^{\frac{\left(p^i_I\right)^2}{t}}\mathrm{e}^{-\frac{\pi^2\left(N^i_I\right)^2+2\pi\mathrm{i}N^i_I p^i_I}{t}} =: \prod_{\substack{e_I\in E(\gamma)\\ i\in 1,2,3}} 2\pi\sqrt{\frac{\pi}{t}}\,\mathrm{e}^{\frac{\left(p^i_I\right)^2}{t}}(1+K_t), \tag{10.15}$$

where K_t is of order $\mathcal{O}(t^\infty)$, meaning we can neglect it when considering the limit $t \to 0$. This is a crucial point that we will heavily make us of: An increasingly smaller classicality parameter t will steadily squeeze the Gaussian functions more and more until, effectively, only terms with $N^i_I = 0$ contribute.

A straightforward analytical computation of expectation values like (10.14) is, however, still not feasible and we are in need further techniques. We already mentioned that there are two branches: Proceeding with estimates and obtain approximative results, or choose special scenarios that then indeed allow an analytical calculation.

Chapter 11

Kummer's confluent hypergeometric functions

This is the key ingredient we will work with in both the analytic branch as well as during the approximative approach — at least for some ansätze there. We start with describing the origin and definition of these special functions and then introduce those properties that we will use during our investigations. Afterwards, we explain the general integration procedure via Kummer's confluent hypergeometric functions by taking the example of quantum mechanics.

Kummer's confluent hypergeometric functions — which we will abbreviate as KCHFs — originate as solutions to Kummer's differential equation [219]

$$z\frac{\mathrm{d}^2 w}{\mathrm{d}z^2} + (b - z)\frac{\mathrm{d}w}{\mathrm{d}z} - aw = 0. \tag{11.1}$$

This equation has two independent solutions, which are straightforwardly referred to as Kummer functions of the first and of the second kind, respectively. Denoting the Kummer function of the first kind by ${}_1\mathrm{F}_1(a, b, z)$ and that of the second kind by $U(a, b, z)$, they read

$${}_1\mathrm{F}_1(a, b, z) \coloneqq \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n n!} z^n \text{ and} \tag{11.2}$$

$$U(a, b, z) \coloneqq \frac{\Gamma(1-b)}{\Gamma(1+a-b)}{}_1\mathrm{F}_1(a, b, z) + \frac{\Gamma(b-1)}{\Gamma(a)} z^{1-b}{}_1\mathrm{F}_1(1+a-b, 2-b, z). \tag{11.3}$$

We will call z the *argument* of ${}_1\mathrm{F}_1(a,b,z)$, while referring to a and b as its *parameters*. The quantities $(a)_n$ therein are the *Pochhammer symbol*, also named the rising factorial:

$$
\begin{aligned}
(a)_0 &= 1, \\
(a)_1 &= a \quad \text{and} \\
(a)_n &= a(a+1)(a+2)\cdots(a+n-1). \qquad (11.4)
\end{aligned}
$$

When it comes to the naming of special functions and accompanied notations, however, the literature offers a vast amount of different choices. We use those that became — to our best knowledge — the established standard over time, but the interested reader may find other ones, too: Initially, Kummer used $\varphi(\alpha,\beta,x)$ instead of ${}_1\mathrm{F}_1(a,b,z)$ in [219, cf. e.g. eq. 1.], while it is nowadays often symbolised by $M(a,b,z)$. This should not be confused with the regularised KCHF $\mathrm{M}(a,b,z)\,\Gamma(b) \coloneqq M(a,b,z)$, denoted by an upright M, which is often used due its advantageous avoidance of the KCHFs' singularities when b is 0 or a negative integer. The Kummer functions of the second kind, $U(a,b,z)$, are in turn sometimes also referred to as Tricomi's functions, named after Francesco Tricomi who introduced them in [220]. Lastly, also the Pochhammer symbol offers a similar variety of labellings: You may find it in the literature as $a^{(n)}$ or $a^{\overline{n}}$, while Pochhammer himself denoted it by $[a]_n^+$, confer [221, p. 80-81]. Therein, you will also find $(a)_n$, which he, however, used for the binomial coefficient $\binom{a}{n}$. Note that $(a)_n$ is sometimes even used not for the rising but the falling factorial — one really has to pay attention to the context when seeing any of those symbols. When we later use the falling factorial, we will use $(a)_n^-$ to stick to the logics of the Pochhammer symbol, while you will mostly find $a^{\underline{n}}$ in the literature.

Kummer's functions ${}_1\mathrm{F}_1(a,b,z)$ are entire functions in a and z, while they are meromorphic functions in b: they experience the aforementioned poles in $b = -n \,\forall\, n \in \mathbb{N}_0$. Note that $\mathrm{M}(a,b,z)$ is therefore an entire function of all a, z and b. Kummer's function of the second kind has a branch point at $z = 0$ and is otherwise entire in a and b. KCHFs include numerous elementary functions via particular choices of their parameters, like

$$ {}_1\mathrm{F}_1(0,b,z) = 1, \tag{11.5} $$

$$ {}_1\mathrm{F}_1(a,a,z) = \mathrm{e}^z, \tag{11.6} $$

$$ U\Big(-\frac{r}{2},-\frac{r}{2},x^2\Big) = \big(x^2\big)^{\frac{r}{2}} = |x|^r, \tag{11.7} $$

$$U\left(-\frac{n}{2}, \frac{1}{2}, z^2\right) = 2^n H_n(z) \quad \text{with the Hermite polynomials } H_n(z) \tag{11.8}$$

and many further ones, including links to Bateman's function, Bessel functions, Laguerre polynomials etc. [222, 223]. Kummer's confluent hypergeometric function for its part can be seen as a special limit of the (ordinary) Gaussian hypergeometric function ${}_2\mathrm{F}_1(a, c; b; z)$:

$${}_1\mathrm{F}_1(a, b, z) = \lim_{c\to\infty} {}_2\mathrm{F}_1\left(a, c; b; \frac{z}{c}\right), \text{ where} \tag{11.9}$$

$${}_2\mathrm{F}_1(a, c; b; z) := \sum_{n=0}^{\infty} \frac{(a)_n (c)_n}{(b)_n n!} z^n. \tag{11.10}$$

We end the general introduction of Kummer's functions with an an important property, the so-called Kummer's transformations

$${}_1\mathrm{F}_1(a, b, z) = \mathrm{e}^z \, {}_1\mathrm{F}_1(b-a, b, -z) \quad \text{and} \tag{11.11}$$

$$U(a, b, z) = z^{1-b} U(a-b-1, 2-b, z), \tag{11.12}$$

which we will use quite frequently during our calculations. The upcoming two subsections introduce two further properties in some more detail as they are key techniques for the subsequent computations.
In Appendix A, we also offer a brief biographical overview over the influential life and work of Ernst Eduard Kummer.

11.1 The Fourier transformation

The first of those properties is about the Fourier transformation. It turns out that the Kummer functions of the first and second kind can be transferred from one to the other via Fourier transformations including Gaussian functions. So to some extend, the two Kummer functions are dual to each other. This result was published by Pichler in [210, Theorem 3] and its proof relies on another theorem therein, [210, Theorem 1], namely the "Expansion of Kummer's functions in terms of Laguerre polynomials". Adopted to our notation, the relevant part of [210, Theorem 3] for our purpose reads:

Theorem 1 (Pichler) *(Fourier transform of Kummer's functions). Kummer's functions are symmetric with respect to Fourier transformation. Let $x, k \in \mathbb{R}$, we have for* $\mathrm{Re}(b-a) > 0$

$$\mathcal{F}\Big(\mathrm{e}^{-x^2} U\big(a,b,x^2\big)\Big) = \frac{1}{\sqrt{2}} \frac{\Gamma\big(\frac{3}{2}-b\big)}{\Gamma\big(a-b+\frac{3}{2}\big)}\ \mathrm{e}^{-\frac{k^2}{4}}\,{}_1\mathrm{F}_1\left(a, a+\frac{3}{2}-b, \frac{k^2}{4}\right) \text{ and} \tag{11.13}$$

$$\mathcal{F}\Big(\mathrm{e}^{-x^2}\,{}_1\mathrm{F}_1\big(a,b,x^2\big)\Big) = \frac{1}{\sqrt{2}} \frac{\Gamma(b)}{\Gamma(b-a)}\ \mathrm{e}^{-\frac{k^2}{4}} U\left(a, a+\frac{3}{2}-b, \frac{k^2}{4}\right). \tag{11.14}$$

Therein, we used

$$\mathcal{F}[f](k) := \hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}x\, f(x)\ \mathrm{e}^{-\mathrm{i}kx} \quad\text{and}\quad \mathcal{F}^{-1}[\hat{g}](x) := g(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}k\, \hat{g}(k)\ \mathrm{e}^{\mathrm{i}kx}$$

for the one-dimensional Fourier transformation $\mathcal{F}[f]$, or $\hat{f}$, and its inverse $\mathcal{F}^{-1}[\hat{f}]$. However, for our purpose, we work with a slightly modified version of this theorem, which was introduced in [2]:

Lemma 1 *Let $x, k \in \mathbb{R}, \mathrm{Re}(b-a) > 0$ and $\alpha \in \mathbb{C}$. Then, we have*

$$\mathcal{F}\Big(\mathrm{e}^{-x^2} U\big(a,b,x^2\big)\mathrm{e}^{\mathrm{i}\alpha x}\Big) = \frac{1}{\sqrt{2}} \frac{\Gamma\big(\frac{3}{2}-b\big)}{\Gamma\big(a-b+\frac{3}{2}\big)}\ \mathrm{e}^{-\frac{(k-\alpha)^2}{4}}\,{}_1\mathrm{F}_1\left(a, a+\frac{3}{2}-b, \frac{(k-\alpha)^2}{4}\right) \text{ and} \tag{11.15}$$

$$\mathcal{F}\Big(\mathrm{e}^{-x^2}\,{}_1\mathrm{F}_1\big(a,b,x^2\big)\mathrm{e}^{\mathrm{i}\alpha x}\Big) = \frac{1}{\sqrt{2}} \frac{\Gamma(b)}{\Gamma(b-a)}\ \mathrm{e}^{-\frac{(k-\alpha)^2}{4}} U\left(a, a+\frac{3}{2}-b, \frac{(k-\alpha)^2}{4}\right). \tag{11.16}$$

It essentially follows from the modulation property of the Fourier transformation itself:

$$\mathcal{F}(\mathrm{e}^{\mathrm{i}k_0 x} f(x)) = \hat{f}(k-k_0). \tag{11.17}$$

11.2 The asymptotic expansion for large arguments

The second property will be of paramount importance during our semiclassical considerations: the *asymptotic expansion for large arguments of the KCHF*. For $|z| \to \infty$, we have [222]

$$
{}_1\mathrm{F}_1(a,b,z) \overset{|z|\to\infty}{\approx} \Gamma(b)\left[\frac{\mathrm{e}^{\pm\pi\mathrm{i}a} z^{-a}}{\Gamma(b-a)} \sum_{n=0}^{\infty} \frac{(a)_n(1+a-b)_n}{n!}(-z)^{-n} + \right.
$$
$$
\left. + \frac{\mathrm{e}^z z^{a-b}}{\Gamma(a)} \sum_{n=0}^{\infty} \frac{(b-a)_n(1-a)_n}{n!} z^{-n}\right], \tag{11.18}
$$

where we need to choose the minus sign in $\exp(\pm\pi\mathrm{i}a)$ if z lies in the right half plane [222]. A similar expansion is also available for the Kummer function of the second kind, reading

$$
U(a,b,z) \overset{|z|\to\infty}{\approx} z^{-a} \sum_{n=0}^{\infty} \frac{(a)_n(1+a-b)_n}{n!}(-z)^{-n}. \tag{11.19}
$$

Note that we now use the symbol $\approx$ to highlight approximations like applying one of the asymptotic expansion formulae.

11.3 The procedure — exemplified by quantum mechanics

In this section, we will use familiar quantum mechanics and its coherent states to introduce the general idea of the procedure that we will later use in the $\mathrm{U}(1)^3$-scenario. We start by computing semiclassical expectation values of fractional powers of the momentum operator, $|\hat{p}|^r$, and then proceed to an operator that we can use to mimic the $\hat{q}^{i_0}_{I_0}(r)$-operator of loop quantum gravity.

The way KCHFs will enter our calculations most times is via one of the two integrals

$$
\int_{-\infty}^{\infty} \mathrm{e}^{-\rho^2(x-\mu)^2} |x|^r \mathrm{d}x = |\rho|^{-1-r}\, \Gamma\left(\frac{r+1}{2}\right) {}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, -\rho^2\mu^2\right) \quad \text{or} \tag{11.20}
$$
$$
\int_{-\infty}^{\infty} \mathrm{e}^{-\rho^2x^2+2\rho^2\mu x} |x|^r \mathrm{d}x = |\rho|^{-1-r}\Gamma\left(\frac{r+1}{2}\right) {}_1\mathrm{F}_1\left(\frac{r+1}{2}, \frac{1}{2}, \rho^2\mu^2\right), \tag{11.21}
$$

where $\mathrm{Re}(r) > -1$ and $\mathrm{Re}(\rho^2) > 0$. First of all, these two identities are, of course, related.

Via the Kummer transformation (11.11), we can rewrite

$$ {}_1\mathrm{F}_1\Big(-\frac{r}{2},\frac{1}{2},-\rho^2\mu^2\Big) = \mathrm{e}^{-\rho^2\mu^2}\,{}_1\mathrm{F}_1\Big(\frac{1+r}{2},\frac{1}{2},\rho^2\mu^2\Big) \tag{11.22} $$

and obtain a link between the respective right hand sides of (11.20) and (11.21). The additional Gaussian can now be used to complete the square on the left hand side of (11.21) and we see the two identities do indeed describe the same integration procedure.

We can also understand these two formulae via the generalised Lemma 1 we introduced in Section 11.1. Using (11.7),

$$ |x|^r = \big(x^2\big)^{\frac{r}{2}} = U\Big(-\frac{r}{2},-\frac{r}{2},x^2\Big), \tag{11.23} $$

gives rise to the Kummer function of the second kind within the integrand of both (11.20) and (11.21) and we can indeed apply Lemma 1 to both.

Now, when it comes to classical quantum mechanics, the coherent states take the well-known form

$$ \Psi_{\mathrm{coh}} = \Psi^{\hbar}_{q,p} = \frac{1}{\sqrt[4]{\pi}\sqrt{\sigma}}\;\mathrm{e}^{-\frac{(x-q)^2}{2\sigma^2}}\;\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \tag{11.24} $$

in the position representation. Therein, the subscript q,p highlights that the state is peaked around (q,p) in phase space, while the superscript $\hbar$ labels the state as being a quantum mechanical one — as opposed to the coherent states of SU(2) or $\mathrm{U}(1)^3$. We collect all constants in $\sigma \coloneqq \sqrt{\frac{\hbar}{m\omega}}$, which also corresponds to the width of the coherent state in phase space. As already stated, we start with computing the expectation value of fractional powers of the momentum operator, i.e.

$$ \langle|\hat{p}|^r\rangle_{\Psi^{\hbar}_{q,p}} = \langle\Psi^{\hbar}_{q,p}\,|\,|\hat{p}|^r\,|\,\Psi^{\hbar}_{q,p}\rangle = \int_{-\infty}^{\infty} \mathrm{d}k\,\mathcal{F}[\overline{\Psi^{\hbar}_{q,p}}](k)\,|k|^r\,\mathcal{F}[\Psi^{\hbar}_{q,p}](k) \tag{11.25} $$

$$ \text{with } r\in\mathbb{Q}\wedge r>-\frac{1}{2}. $$

While the integral above is well-defined for $r>-1$ already, we further constrain $r>-\frac{1}{2}$ as this additionally implies that $|\hat{p}|^r\Psi^{\hbar}_{q,p}$ is normalisable. For the last identity above, we used that the momentum operator acts diagonally on the (generalised) momentum eigenstates of quantum mechanics, which we put into the expression via a resolution of identity. We can now use the already mentioned modulation property of the Fourier transform as well as the the self-reciprocity of Gaussian functions under Fourier transformations and obtain

$$\langle |\hat{p}|^r \rangle_{\Psi^{\hbar}_{q,p}} = \frac{\sigma}{\hbar\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \mathrm{d}k \big(k^2\big)^{\frac{r}{2}} \mathrm{e}^{-\frac{\sigma^2}{\hbar^2}(k-p)^2} = \frac{\sigma}{\sqrt{\pi}\hbar} \mathrm{e}^{\left(\frac{\sigma}{\hbar}p\right)^2} \int\limits_{-\infty}^{\infty} \mathrm{d}k \big(k^2\big)^{\frac{r}{2}} \mathrm{e}^{-\left(\frac{\sigma}{\hbar}k\right)^2} \mathrm{e}^{\mathrm{i}\left(-2\mathrm{i}\frac{\sigma}{\hbar}p\right)\frac{\sigma}{\hbar}k}. \tag{11.26}$$

The last identity therein was introduced as a preparation for applying Lemma 1. We already have the exponential function and what is left is replacing $|k|^r$ by a KCHF. Using (11.23) we find

$$\langle |\hat{p}|^r \rangle_{\Psi^{\hbar}_{q,p}} = \frac{\sigma}{\hbar\sqrt{\pi}} \mathrm{e}^{\left(\frac{\sigma}{\hbar}p\right)^2} \left(\frac{\hbar}{\sigma}\right)^r \int\limits_{-\infty}^{\infty} \mathrm{d}k\, U\left(-\frac{r}{2}, -\frac{r}{2}+1, \left(\frac{\sigma}{\hbar}k\right)^2\right) \mathrm{e}^{-\left(\frac{\sigma}{\hbar}k\right)^2} \mathrm{e}^{\mathrm{i}\left(-2\mathrm{i}\frac{\sigma}{\hbar}p\right)\frac{\sigma}{\hbar}k}. \tag{11.27}$$

Therefore, we can now indeed apply Lemma 1:

$$\frac{\sqrt{2}\Gamma\left(\frac{r+1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \frac{\hbar}{2\sigma} \mathcal{F}\left(\mathrm{e}^{-\left(\frac{\hbar x}{2\sigma}\right)^2} {}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, \left(\frac{\hbar x}{2\sigma}\right)^2\right)\right) = U\left(-\frac{r}{2}, -\frac{r}{2}+1, \left(\frac{\sigma}{\hbar}k\right)^2\right) \mathrm{e}^{-\left(\frac{\sigma}{\hbar}k\right)^2}. \tag{11.28}$$

Putting all those ingredients together, we get

$$\begin{aligned} \langle \Psi^{\hbar}_{q,p} \,|\, |\hat{p}|^r \,|\, \Psi^{\hbar}_{q,p} \rangle &= \frac{\Gamma\left(\frac{r+1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \left(\frac{\hbar}{\sigma}\right)^r \mathrm{e}^{\frac{\sigma^2}{\hbar^2}p^2} \mathcal{F}^{-1}\left[\mathcal{F}\left[\mathrm{e}^{-\left(\frac{\hbar x}{2\sigma}\right)^2} {}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, \left(\frac{\hbar x}{2\sigma}\right)^2\right)\right]\right] \\ &= \frac{\Gamma\left(\frac{r+1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \left(\frac{\hbar}{\sigma}\right)^r \mathrm{e}^{\frac{\sigma^2}{\hbar^2}p^2} \mathrm{e}^{-\left(\frac{\sigma p}{\hbar}\right)^2} {}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, -\left(\frac{\sigma p}{\hbar}\right)^2\right) \\ &= \frac{\Gamma\left(\frac{r+1}{2}\right)}{\sqrt{\pi}} \left(\frac{\hbar}{\sigma}\right)^r {}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, -\left(\frac{\sigma p}{\hbar}\right)^2\right) \end{aligned} \tag{11.29}$$

and see that we reproduced (11.20) to obtain the expectation value of $|\hat{p}|^r$ with respect to coherent states — namely a Kummer function of the first kind. A quick check for $r = 0$ recovers the normalisation of the coherent states via ${}_1\mathrm{F}_1\left(0, \frac{1}{2}, -\left(\frac{\sigma p}{\hbar}\right)^2\right) = 1$. Also, when it comes to the applicability of Lemma 1, we need to ensure $\mathrm{Re}(b-a) > 0$ for the involved KCHFs. With constraining $r > -\frac{1}{2}$, this is fulfilled for both ${}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, .\right)$ and $U\left(-\frac{r}{2}, \frac{r}{2}+1, .\right)$.

Note that this was a completely analytical computation, without the need of estimates or performing a Taylor expansion. However, as a final result, (11.29) is still a bit unsatisfying and this is where the previously introduced asymptotic expansion for large arguments of the KCHF, (11.18), comes into play. Working in quantum mechanics, we have with $\hbar$

a parameter at hand that can be used to tell whether a quantity can be considered as being small or, via inverse powers of it, in fact large. In the final result of (11.29) above, the argument of the KCHF reads $z = -\left(\frac{\sigma p}{\hbar}\right)^2 = -\frac{p^2}{\hbar m \omega}$ and we can therefore indeed apply the expansion for large arguments:

$$\begin{aligned}\langle \Psi^{\hbar}_{q,p} \,|\, |\hat{p}|^r \,|\, \Psi^{\hbar}_{q,p} \rangle &\approx \frac{\Gamma\left(\frac{r+1}{2}\right)}{\sqrt{\pi}} \left(\frac{\hbar}{\sigma}\right)^r \Gamma\left(\tfrac{1}{2}\right) \left[\frac{\mathrm{e}^{\mp \pi \mathrm{i} \frac{r}{2}} \left(-\frac{p^2}{\hbar m \omega}\right)^{\frac{r}{2}}}{\Gamma\left(\frac{r+1}{2}\right)} \sum_{n=0}^{\infty} \frac{\left(-\frac{r}{2}\right)_n \left(\frac{1-r}{2}\right)_n}{n!} \left(\frac{\hbar m \omega}{p^2}\right)^n + \right. \\ &\quad \left. + \frac{\mathrm{e}^{-\frac{p^2}{\hbar m \omega}} \left(-\frac{p^2}{\hbar m \omega}\right)^{-\frac{1+r}{2}}}{\Gamma\left(-\frac{r}{2}\right)} \sum_{n=0}^{\infty} \frac{\left(\frac{1+r}{2}\right)_n \left(1+\frac{r}{2}\right)_n}{n!} \left(-\frac{\hbar m \omega}{p^2}\right)^n \right] \\ &\approx |p|^r \sum_{n=0}^{\infty} \frac{\left(-\frac{r}{2}\right)_n \left(\frac{1-r}{2}\right)_n}{n!} \left(\frac{\hbar m \omega}{p^2}\right)^n \\ &\approx |p|^r \left(1 - \frac{r(1-r)}{4} \frac{\hbar m \omega}{p^2} + \mathcal{O}\left(\hbar^2\right)\right). \end{aligned} \tag{11.30}$$

Therein, a computationally advantageous feature of the asymptotic expansion was used that we will always face in our considerations: Out of the two sums of the asymptotic expansions, one generically vanishes due to a remaining Gaussian prefactor that damps that contribution to $\mathcal{O}(\hbar^\infty)$. In the above, this is the case for the second sum, which is preceded by the Gaussian function $\mathrm{e}^{-\frac{p^2}{\hbar m \omega}}$. Next, we have a minus sign in the exponential function within the first sum as the argument of the KCHF is negative and $a = -\frac{r}{2}$. Together with the fractional power of -1 within the prefactor $\left(-\frac{p^2}{\hbar m \omega}\right)^{\frac{r}{2}}$, this completes to $\mathrm{e}^{-\pi \mathrm{i} \frac{r}{2}} (-1)^{\frac{r}{2}} = (-1)^{-\frac{r}{2}} (-1)^{\frac{r}{2}} = 1$ and there is no imaginary part left — as it should be. Thereby, we end up with a series expansion that is calculable up to any desired order and which also reproduces the expected zeroth order result $|p|^r$.

We now proceed to an operator that we use to mimic the class of $\mathrm{U}(1)^3$-operators $\hat{q}^{i_0}_{I_0}(r)$ in quantum mechanics:

$$\hat{q}_{\mathrm{qm}}(r) = \mathrm{e}^{\mathrm{i}\alpha\hat{x}} \left[\mathrm{e}^{-\mathrm{i}\alpha\hat{x}}, |\hat{p}|^r\right] = |\hat{p}|^r - \mathrm{e}^{\mathrm{i}\alpha\hat{x}} |\hat{p}|^r \mathrm{e}^{-\mathrm{i}\alpha\hat{x}}. \tag{11.31}$$

With the volume operator depending on the fluxes, recap (2.106), it is a straightforward choice to choose the momentum operator as representative in the quantum mechanical toy model. The exponent r is then used to get the correct power. As equivalent of the holonomy operator, we introduced $\mathrm{e}^{\mathrm{i}\alpha\hat{x}}$. If we single out the last e-function $\mathrm{e}^{\frac{\mathrm{i}}{\hbar} p x}$ within the definition of the quantum mechanical coherent states, (11.24), we can combine it with $\mathrm{e}^{\mathrm{i}\alpha x}$, the action of the holonomy-like quantum mechanical operator, to obtain a shifted momentum $p \mapsto p - \hbar\alpha$. This is also how the holonomy operator acts in U(1), so the choice does indeed make sense.

We will now perform the calculations for the choice of r that, in $\mathrm{U}(1)^3$, reflects the scenario where $\hat{q}^{i_0}_{I_0}(r)$ contains the square root of the volume operator — which is a frequently appearing quantity in loop quantum gravity. Recap that the volume operator (2.106) is essentially the square root of the operator $\hat{\mathrm{Q}}_v$, (2.107), which in turn is proportional to the product of three fluxes. Interpreting the momentum operator as the quantum mechanical equivalent of the fluxes in loop quantum gravity, we are therefore left with the association $\sqrt{\hat{\mathrm{V}}}\Big|_{\mathrm{lqg}} \mapsto |p|^{\frac{3}{4}}\Big|_{\mathrm{qm}}$ and the expectation value of interest reads

$$\langle|\hat{q}_{\mathrm{qm}}(r)|^r\rangle_{\Psi^\hbar_{q,p}} = \langle\Psi^\hbar_{q,p}|\mathrm{e}^{\mathrm{i}\alpha\hat{x}}\left[\mathrm{e}^{-\mathrm{i}\alpha\hat{x}}, \sqrt[4]{|\hat{p}|^3}\right]|\Psi^\hbar_{q,p}\rangle. \tag{11.32}$$

We can compute this in two steps, referring to our previous result for $\langle|\hat{p}|^r\rangle_{\Psi^\hbar_{q,p}}$, (11.29). With one of the two contributions being precisely the result of (11.29) for $r = \frac{3}{4}$, we have

$$\langle\sqrt[4]{|\hat{p}|^3}\rangle_{\Psi^\hbar_{q,p}} = \frac{1}{\sqrt{\pi}}\left(\frac{\hbar}{\sigma}\right)^{\frac{3}{4}}\Gamma\big(\tfrac{7}{8}\big)\,{}_1\mathrm{F}_1\left(-\frac{3}{8}, \frac{1}{2}, -\frac{\sigma^2}{\hbar^2}p^2\right). \tag{11.33}$$

As we already associated the action of the holonomy-like operator as a shift in the momentum only, we can also directly deduce

$$\langle\sqrt[4]{|\hat{p}|^3}\rangle_{\mathrm{e}^{-\mathrm{i}\alpha\hat{x}}\Psi^\hbar_{q,p}} = \frac{1}{\sqrt{\pi}}\left(\frac{\hbar}{\sigma}\right)^{\frac{3}{4}}\Gamma\big(\tfrac{7}{8}\big)\,{}_1\mathrm{F}_1\left(-\frac{3}{8}, \frac{1}{2}, -\frac{\sigma^2}{\hbar^2}(p-\hbar\alpha)^2\right). \tag{11.34}$$

The arguments of the KCHFs in both contributions go with $-\frac{\sigma^2}{\hbar^2}p^2 = -\frac{p^2}{m\omega\hbar}$, i.e. with $\frac{1}{\hbar}$ in at least one of their terms. We can therefore apply the asymptotic expansion for large arguments, (11.18), and get

$$\begin{aligned}\langle\Psi^\hbar_{q,p}|\mathrm{e}^{\mathrm{i}\alpha\hat{x}}\left[\mathrm{e}^{-\mathrm{i}\alpha\hat{x}}, \sqrt[4]{|\hat{p}|^3}\right]|\Psi^\hbar_{q,p}\rangle &\approx \frac{3}{4}\frac{\alpha|p|^{\frac{3}{4}}}{p}\hbar + \left(\frac{3}{32}\frac{\alpha^2|p|^{\frac{3}{4}}}{p^2} + \frac{15}{256}\frac{\alpha m\omega|p|^{\frac{3}{4}}}{p^3}\right)\hbar^2 \\ &+ \left(\frac{5}{128}\frac{\alpha^3|p|^{\frac{3}{4}}}{p^3} + \frac{135}{2048}\frac{\alpha^2 m\omega|p|^{\frac{3}{4}}}{p^4} + \frac{1755}{32768}\frac{\alpha m^2\omega^2|p|^{\frac{3}{4}}}{p^5}\right)\hbar^3 + \mathcal{O}\big(\hbar^4\big).\end{aligned} \tag{11.35}$$

Just like before, we were able to drop one sum per expansion due to damping Gaussian prefactors.[1] The lowest order contribution divided by $\hbar$ matches the result one obtains for the Poisson bracket of the classical counterparts of the involved operators. In the next section, we will try to replicate this result by means of a different approach to semiclassical analyses from the literature.

Before, we also want to address the case $p = 0$ as we notice that the result above would diverge did we take that limit. Setting $p = 0$ in (11.33) & (11.34), we immediately see that we have to proceed differently from thereon anyway. With $p = 0$, the argument of the KCHF within (11.33) vanishes, yielding ${}_1\mathrm{F}_1(a, b, 0) = 1$. For (11.34) with $p = 0$, in turn, we can use the non-approximative series expansion of the KCHF, (11.2), and directly obtain a power series in $\hbar$:

$$\begin{aligned}\langle\Psi^{\hbar}_{q,p}|\mathrm{e}^{\mathrm{i}\alpha\hat{x}}\left[\mathrm{e}^{-\mathrm{i}\alpha\hat{x}}, \sqrt[4]{|\hat{p}|^3}\right]|\Psi^{\hbar}_{q,p}\rangle &\overset{p=0}{=} \frac{1}{\sqrt{\pi}}(\hbar m\omega)^{\frac{3}{8}}\Gamma\left(\tfrac{7}{8}\right)\left(1 - \sum_{n=0}^{\infty}\frac{\left(-\frac{3}{8}\right)_n}{\left(\frac{1}{2}\right)_n n!}\left(-\frac{\alpha\hbar}{m\omega}\right)^n\right) \\ &= -\frac{3\Gamma\left(\frac{7}{8}\right)}{4\sqrt{\pi}}\frac{\alpha^2}{(m\omega)^{\frac{5}{8}}}\hbar^{\frac{11}{8}} + \mathcal{O}\left(\hbar^{\frac{19}{8}}\right). \end{aligned} \tag{11.36}$$

So we do in fact not end up with a diverging expression for the limit $p = 0$ after all.

11.4 Comparison with the algebraic quantum gravity approach

We now want to compare the previously obtained analytical result for the semiclassical expectation value with an approximative method from the literature. This procedure originates from the previously introduced framework called *algebraic quantum gravity*, introduced by Giesel and Thiemann in [58–61]. In the third paper of this series, [60], they show that one can replace the operator of interest, i.e. which one aims to compute semiclassical expectation values of, by a power series in the classicality parameter that only contains integer powers of operators one can in turn compute expectation values of. So starting with an operator to the power of $r \in \mathbb{Q}$, one ends up with a power series in expectation values of that operator to the power of $n \in \mathbb{N}$. In our case, this operator is $\hat{\mathrm{Q}}_v$: If we want to compute semiclassical expectation values of $\hat{q}^{i_0}_{I_0}(r)$ in loop quantum

[1] Note that we could have used just as well the final result after performing the expansion, (11.30).

gravity, which include $\hat{\mathrm{V}}^r$, it ultimately means to compute semiclassical expectation values of $\left(\hat{\mathrm{Q}}_v\right)^{\frac{r}{2}}$. We motivated that this is not analytically possible in full generality, but via the method of [60], we end up with computing integer powers $\left(\hat{\mathrm{Q}}_v\right)^n, n \in \mathbb{N}$, only. The actual replacement of the volume operator to the power of a rational number within the semiclassical expectation value with respect to Ψ by a power series then looks like [60]

$$\hat{\mathrm{V}}_v^{4q} \mapsto \left(\langle \hat{\mathrm{Q}}_v \rangle_\Psi\right)^{2q} \left(1 + \sum_{n=1}^{2k+1} (-1)^{n+1} \frac{q(1-q)\cdots(n-1-q)}{n!} \left(\frac{\hat{\mathrm{Q}}_v^2}{\langle \hat{\mathrm{Q}}_v \rangle_\Psi^2} - 1\right)^n\right), \tag{11.37}$$

which is correct up to the order $\hbar^{k+1}$.

We now apply this technique to the toy model of semiclassical expectation values of (11.31) within quantum mechanics. As before, we consider the square root of the volume operator, meaning $r = \frac{1}{2}$, and for the power series above we choose $k = 1$, i.e. we include correction terms up to $\sim \hbar^2$. With $k = 1$, we have to compute expectation values of powers of $\hat{p}$ up to $\hat{p}^{18}$. However, for integer powers we can use the standard techniques and end up with

$$\langle \mathrm{e}^{\mathrm{i}\alpha\hat{x}} \left[\mathrm{e}^{-\mathrm{i}\alpha\hat{x}}, \sqrt[4]{|\hat{p}|^3}\right] \rangle_{\Psi^\hbar_{q,p}} \approx \frac{3}{4}\frac{\alpha|p|^{\frac{3}{4}}}{p}\hbar + \left(\frac{3}{32}\frac{\alpha^2|p|^{\frac{3}{4}}}{p^2} + \frac{15}{256}\frac{\alpha m\omega|p|^{\frac{3}{4}}}{p^3}\right)\hbar^2 + \mathcal{O}\big(\hbar^3\big). \tag{11.38}$$

Comparing this result with the previously obtained one via KCHFs, (11.35), we realise that they do indeed agree.

Chapter 12

Kummer's functions and coherent states on the circle

Before we delve into the computation of semiclassical expectation values via Kummer's confluent hypergeometric functions in loop quantum gravity, we use this chapter to investigate coherent states on the circle in the light of Kummer's functions. In the literature, coherent states on the circle were investigated so far either via the complexifier method [208] or using the so-called Zak transform [204–207]. This chapter now aims at combining these two approaches and Kummer's confluent hypergeometric functions help computing semiclassical expectation values.

12.1 The Zak transformation

We start with some short remarks along the lines of [224]: The Zak transformation is named after Joshua Zak who introduced it in [209] as the "k-q representation" for describing Bloch electrons in electromagnetic fields. Israïl Gel'fand discovered it already earlier in [225], but it is only rarely found as the "Gel'fand mapping" as it was Zak who started to investigate it in more detail. There exists also a different variety of the Zak transform, named the "Weil–Brezin map" after André Weil[1] [228] and Jonathan Brezin [229]. For this particular map, [230] argues that Carl Friedrich Gauß was already aware of it.

[1]As a side note, it was also André Weil who published the collected work of Ernst Eduard Kummer [226, 227].

With the Zak transformation, we can map functions from $\mathbb{R}$ to the torus $\mathbb{T}^2$:

$$\mathcal{Z}_a\colon L_2(\mathbb{R}) \to L_2(\mathbb{R}^2/\mathbb{Z}^2), \quad f \mapsto \mathcal{Z}_a[f](x,\zeta) := \sqrt{a}\sum_{n=-\infty}^{\infty} f(x+2\pi n a)\mathrm{e}^{-2\pi i n a\zeta}. \tag{12.1}$$

Therein, $\zeta \in [0, 1/a]$ and — in abuse of notation — we use the same $x \in [0, 2\pi a]$ for both the old and new variable. Note that while we work in one dimension only, the Zak transform can also be extended to $L_2(\mathbb{R}^n)$. The corresponding inverse mapping $\mathcal{Z}_a^{-1}\colon L_2(\mathbb{R}^2/\mathbb{Z}^2) \to L_2(\mathbb{R})$ now reads

$$\mathcal{Z}_a^{-1}[g](x) := \sqrt{a}\int_0^{\frac{1}{a}} \mathrm{d}\zeta\, g(x,\zeta), \tag{12.2}$$

with $a \neq 0 \in \mathbb{R}$. After applying the Zak transformation, we obtain with $\mathcal{Z}_a[f]$ a periodic function in ζ that is furthermore quasiperiodic in x:

$$g\big(x, \zeta + \tfrac{\ell}{a}\big) = g(x,\zeta) \quad \text{and} \quad g(x+2\pi a m, \zeta) = \mathrm{e}^{2\pi i m a\zeta} g(x,\zeta) \quad \text{for} \quad g = \mathcal{Z}_a[f],\ \ell, m \in \mathbb{Z}. \tag{12.3}$$

Accordingly, the choice of its values in $[0, 2\pi a] \times [0, \frac{1}{a}]$ fully defines $\mathcal{Z}_a[f]$.

As a short example, we compute the Zak transformation of a Gaussian $f_\mathrm{G}\colon \mathbb{R} \to \mathbb{R}, x \mapsto f_\mathrm{G}(x) := \mathrm{e}^{-\frac{x^2}{4b}}$. To keep the formulae short, we use $a = 1$ and $\mathcal{Z}_1 =: \mathcal{Z}$:

$$\begin{aligned}\mathcal{Z}[f_\mathrm{G}](x,\zeta) &= \sum_{n=-\infty}^{\infty} \mathrm{e}^{-\frac{1}{4b}(x+2\pi n)^2}\mathrm{e}^{-2i\pi n\zeta} \\ &= \mathrm{e}^{-\frac{x^2}{4b}} \sum_{n=-\infty}^{\infty} \mathrm{e}^{2in\left(-\pi\zeta + i2\pi\frac{x}{4b}\right)}\mathrm{e}^{-\frac{(2\pi)^2 n^2}{4b}} \\ &= \mathrm{e}^{-\frac{x^2}{4b}}\Theta\left(-\pi\zeta + \frac{2i\pi x}{4b}, \frac{i\pi}{b}\right).\end{aligned} \tag{12.4}$$

In the last step, we introduced Jacobi's third theta function $\Theta(z, \mathrm{e}^{i\pi\tau}) =: \Theta(z,\tau) := \sum_{n=-\infty}^{\infty} \mathrm{e}^{2inz}\mathrm{e}^{i\pi\tau n^2}$ with $\mathrm{Im}(\tau) > 0$.

We will later also use the combination of the Zak transform of a function and the dilation D_γ of its argument defined as $D_\gamma f(x) := \sqrt{\gamma} f(\gamma x)$ for $\gamma > 0$. Using a result of

[231], the Zak transform of a dilated function reads

$$\mathcal{Z}[D_\gamma f](x,\zeta) = \mathcal{Z}_\gamma[f](\gamma x, \zeta/\gamma), \tag{12.5}$$

where again $\mathcal{Z} := \mathcal{Z}_1$. Associating the two parameters $\gamma = a$, the Zak transformation above becomes

$$\mathcal{Z}_a[f](ax, \zeta/a) = \sqrt{a} \sum_{n=-\infty}^{\infty} f(ax + 2\pi na)\mathrm{e}^{-2\pi \mathrm{i} n\zeta} \tag{12.6}$$

and we will from now on consider the special case of $a = 1$.

As a further example and to get more familiar with the Zak transformation, we show its unitarity following [211]. For $f \in L_1(\mathbb{R}) \cap L_2(\mathbb{R})$,

$$\int_{\mathbb{R}} \mathrm{d}x |f(x)|^2 = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \int_{2\pi k+[0,2\pi]} \mathrm{d}x |f(x)|^2 = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}x \sum_{k=-\infty}^{\infty} |f(x+2\pi k)|^2 < \infty \tag{12.7}$$

holds. The first step consists of a partition of $\mathbb{R}$ into intervals of $[0, 2\pi]$. We then applied Fubini's theorem and lastly used that $f \in L_2(\mathbb{R})$. Hence, $\sum_{k=-\infty}^{\infty} |f(x+2\pi k)|^2 < \infty$ for a.e. $x \in \mathbb{R}$ and the Fourier series $\sum_{k=-\infty}^{\infty} f(x+2\pi k)\ \mathrm{e}^{-2\mathrm{i}\pi k\zeta}$ is well-defined for $f \in L_1(\mathbb{R}) \cap L_2(\mathbb{R})$. We also have

$$\int_0^1 \mathrm{d}\zeta |\mathcal{Z}(x,\zeta)|^2 = \sum_{k=-\infty}^{\infty} |f(x+2\pi k)|^2 \tag{12.8}$$

and with an additional integration over x combined with Fubini's theorem, we end up with

$$\|\mathcal{Z}[f]\|^2_{L_2(\mathbb{R}^2/\mathbb{Z}^2)} = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}x \int_0^1 \mathrm{d}\zeta |\mathcal{Z}(x,\zeta)|^2 \tag{12.9}$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}x \sum_{k=-\infty}^{\infty} |f(x+2\pi k)|^2 = \int_{\mathbb{R}} \mathrm{d}x |f(x)|^2 = \|f\|^2_{L_2(\mathbb{R})}, \tag{12.10}$$

from which we can now deduce the unitarity of the Zak transform as $L_1(\mathbb{R}) \cap L_2(\mathbb{R})$ is dense in $L_2(\mathbb{R})$.

We previously saw that the image of a Gaussian function under the Zak transformation is a theta function. The Zak transform can, however, also be generalised to be applicable to distributions [211]. This results in a bijection between $\mathcal{S}'(\mathbb{R})$ and $\mathcal{Q}'(\mathbb{R}^2)$ — the dual of the Schwartz space and the dual of the space of all quasiperiodic (as in (12.3)) smooth functions.

We now turn towards the complexifier procedure for constructing coherent states, which we already discussed in Section 2.7. Viewed from a different angle, this mechanism constructs coherent states like (11.24) by analytically continuing the heat kernel

$$\rho_t(x,y) = C_{\text{norm}} \frac{1}{\sqrt{t}}\, \mathrm{e}^{-\frac{(x-y)^2}{4k_\mathrm{d} t}}. \tag{12.11}$$

We label the diffusion constant by k_d and the normalisation constant by C_{norm}. To face normalised states, the latter should of course be $C_{\text{norm}} = \frac{1}{\sqrt{4k_\mathrm{d}\pi}}$. Note that Section 12.4 will present more details about the heat equation and self similar solutions thereof. In general, a solution $u(x,t)$ to the heat equation reads

$$u(x,t) = \int_{-\infty}^{\infty} \mathrm{d}y\, \rho_t(x,y) f(y) =: B_{\rho_t}[f](x,t), \tag{12.12}$$

where $f(x)$ describes the boundary conditions and we introduced the so-called Gaussian integral operator $B_\rho \colon \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$ (borrowing the notation of [211]).

The quantum mechanical coherent states can then be obtained via

$$\Psi^\hbar_{q,p}(x) = [\rho_\hbar(x,y)]_{y\to q+\mathrm{i}p} = C_{q,p,\hbar}\, \mathrm{e}^{-\frac{(x-q)^2}{2\hbar}}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}, \tag{12.13}$$

where $C_{q,p,\hbar} := C_{\text{norm}} \exp\big(\frac{1}{2\hbar}(-2\mathrm{i}qp + p^2)\big)$ and $k_\mathrm{d} = \frac{1}{2}, m = 1, \omega = 1$, yielding $\sigma = \sqrt{\hbar}$.

As before, we choose $a = 1$ and obtain [211]

$$\mathcal{Z} B_{\rho_t} \mathcal{Z}^{-1}[g](x,\zeta_1) := \int_0^{2\pi}\int_0^1 \mathcal{K}_{\rho_t}(x,\zeta_1,y,\zeta_2) g(y,\zeta_2)\, \mathrm{d}y\, \mathrm{d}\zeta_2 \tag{12.14}$$

for the Zak transformation $\mathcal{Z} B_{\rho_t} \mathcal{Z}^{-1} \colon \mathcal{Q}(\mathbb{R}^2) \to \mathcal{Q}(\mathbb{R}^2)$ of B_{ρ_t}. For the kernel $\mathcal{K}_{\rho_t}(x,\zeta_1,y,\zeta_2)$, [211] then showed the following link to the Zak transform of the heat kernel:

$$\mathcal{K}_{\rho_t}(x,\zeta_1,y,\zeta_2) = \mathcal{Z}[\rho_t](x,\zeta_1,y,-\zeta_2), \quad (x,\zeta_1),(y,\zeta_2) \in \mathbb{R}^2. \tag{12.15}$$

Note that the minus sign in the fourth argument stems directly from the kernel being a function in $x-y$. With that, we have

$$\begin{aligned}\mathcal{K}_{\rho_t}(x,\zeta_1,y,\zeta_2) &= C_{\text{norm}}\frac{1}{\sqrt{t}}\sum_{n,m=-\infty}^{\infty} \mathrm{e}^{-\frac{(x+2\pi n-y-2\pi m)^2}{4k_\mathrm{d}t}}\mathrm{e}^{-2\mathrm{i}\pi n\zeta_1}\mathrm{e}^{2\mathrm{i}\pi m\zeta_2}\\ &= C_{\text{norm}}\frac{1}{\sqrt{t}}\sum_{n,m=-\infty}^{\infty} \mathrm{e}^{-\frac{(x-y+2\pi(n+m))^2}{4k_\mathrm{d}t}}\mathrm{e}^{-2\mathrm{i}\pi n\zeta_1}\mathrm{e}^{-2\mathrm{i}\pi m\zeta_2},\end{aligned} \tag{12.16}$$

which we now reformulate by means of theta functions. For doing so, we need $\widetilde{n} \coloneqq n+m$ and $\widetilde{m} \coloneqq n-m$ and then get

$$\begin{aligned}\mathcal{K}_{\rho_t}(x,\zeta_1,y,\zeta_2) &= \frac{C_{\text{norm}}}{\sqrt{t}}\sum_{\widetilde{n},\widetilde{m}=-\infty}^{\infty} \mathrm{e}^{\frac{-(x-y+2\pi\widetilde{n})^2}{4k_\mathrm{d}t}}\mathrm{e}^{-2\mathrm{i}\pi\zeta_1\frac{1}{2}(\widetilde{n}+\widetilde{m})}\mathrm{e}^{-2\mathrm{i}\pi\zeta_2\frac{1}{2}(\widetilde{n}-\widetilde{m})}\\ &= \frac{C_{\text{norm}}\,\mathrm{e}^{-\frac{(x-y)^2}{4k_\mathrm{d}t}}}{\sqrt{t}}\sum_{\widetilde{n},\widetilde{m}=-\infty}^{\infty} \mathrm{e}^{-\frac{2\pi\widetilde{n}}{2k_\mathrm{d}t}(x-y)}\mathrm{e}^{-\frac{(2\pi)^2}{4k_\mathrm{d}t}\widetilde{n}^2}\mathrm{e}^{-2\mathrm{i}\pi\widetilde{n}\frac{1}{2}(\zeta_1+\zeta_2)}\mathrm{e}^{-2\mathrm{i}\pi\widetilde{m}\frac{1}{2}(\zeta_1-\zeta_2)}\\ &= \frac{C_{\text{norm}}\,\mathrm{e}^{-\frac{(x-y)^2}{4k_\mathrm{d}t}}}{\sqrt{t}}\Theta\left(-\frac{\pi}{2}(\zeta_1+\zeta_2)+\frac{2\mathrm{i}\pi(x-y)}{4k_\mathrm{d}t},\frac{\mathrm{i}\pi}{k_\mathrm{d}t}\right)\sum_{\widetilde{m}=-\infty}^{\infty}\mathrm{e}^{-2\mathrm{i}\pi\widetilde{m}\frac{1}{2}(\zeta_1-\zeta_2)}.\end{aligned} \tag{12.17}$$

The remaining, non-converging sum above can be cast into

$$\delta(\zeta_2-\zeta_1) = \lim_{n\to\infty}\delta_n(\zeta_1-\zeta_2) = \sum_{\widetilde{m}=-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\widetilde{m}\pi(\zeta_2-\zeta_1)}, \tag{12.18}$$

where

$$\delta_n(\zeta_2-\zeta_1) \coloneqq \sum_{\widetilde{m}=-n}^{n}\mathrm{e}^{\mathrm{i}\widetilde{m}\pi(\zeta_2-\zeta_1)}. \tag{12.19}$$

This leads us to

$$\begin{aligned}&\mathcal{Z}B_{\rho_t}\mathcal{Z}^{-1}[g](x,\zeta_1) =\\ &= \lim_{n\to\infty}\frac{C_{\text{norm}}}{\sqrt{t}}\int_{T^2}\mathrm{d}y\,\mathrm{d}\zeta_2\,\mathrm{e}^{-\frac{(x-y)^2}{4k_\mathrm{d}t}}\Theta\left(-\frac{\pi}{2}(\zeta_1+\zeta_2)+\frac{\mathrm{i}\pi(x-y)}{2k_\mathrm{d}t},\frac{\mathrm{i}\pi}{4k_\mathrm{d}t}\right)\delta_n(\zeta_2-\zeta_1)g(y,\zeta_2).\end{aligned} \tag{12.20}$$

Integrating over ζ_2 and taking the limit $n \to \infty$, we find

$$\begin{aligned} u(x,t,\zeta_1) &:= \mathcal{Z}B_{\rho_t}\mathcal{Z}^{-1}[g](x,\zeta_1) \\ &= \frac{C_{\mathrm{norm}}}{\sqrt{t}} \int\limits_{T^2} \mathrm{d}y\ \mathrm{e}^{-\frac{(x-y)^2}{4k_{\mathrm{d}}t}} \Theta\left(-\pi\zeta_1 + \frac{\mathrm{i}\pi(x-y)}{2k_{\mathrm{d}}t}, \frac{\mathrm{i}\pi}{k_{\mathrm{d}}t}\right) g(y,\zeta_1). \end{aligned} \tag{12.21}$$

Therefore, we have with $u(x,t,\zeta_1) := \mathcal{Z}B_{\rho_t}\mathcal{Z}^{-1}[g](x,\zeta_1)$ a solution of the pushforward of the heat equation by the Zak transform, subject to the quasiperiodic boundary condition $u(x,0,\zeta_1) = \sum_n \mathrm{e}^{-2\mathrm{i}n\pi\zeta_1}\tilde{g}(x,\zeta_1)$. The new $\tilde{g}(x,\zeta)$ includes the normalisation constant C_{norm}. As a check, we may now directly look at the pushforward of the heat equation by the Zak transformation. For the differential $\frac{\partial}{\partial x^j}$, [211] found the pushforward $\mathcal{Z}_*\frac{\partial}{\partial x^j} = \frac{\partial}{\partial x^j}$ — where we again used x for both the old and new coordinates. Accordingly, the pushforwarded heat equation then reads

$$\left(\frac{\partial}{\partial t} - k_{\mathrm{d}}\frac{\partial^2}{\partial x^2}\right) u(x,t,\zeta_1) = 0. \tag{12.22}$$

From this form — with the differential operator part being independent of ζ_1 —, we deduce that $u(x,t,\zeta_1)$ of (12.21) is a solution for any value of ζ_1 and we may as well set $\zeta_1 = 0$. Lastly, we note that ζ_1 corresponds to δ in [205, 207, 208] and k in [206].

This is furthermore in accordance with the convolution property of the Zak transform, shown i.a. in [231]:

$$\forall f_1, f_2 \in L_2(\mathbb{R}), f_1 * f_2 \in L_1(\mathbb{R})\colon \mathcal{Z}[f_1 * f_2] = \mathcal{Z}[f_1] *_y \mathcal{Z}[f_2], \tag{12.23}$$

where

$$(f_1 * f_2)(x) := \int\limits_{\mathbb{R}} \mathrm{d}y\, f_1(x-y) f_2(y), \quad \mathcal{Z}[f_1] *_y \mathcal{Z}[f_2](x,\zeta) := \int\limits_0^1 \mathrm{d}y \mathcal{Z}[f_1](x-y,\zeta)\mathcal{Z}[f_2](y,\zeta). \tag{12.24}$$

We can confirm this consistency check by setting $f_1 = \rho_t$ and $f_2 = g$, with the Zak transformation of ρ_t reading

$$\mathcal{Z}[\rho_t](x-y,\zeta) = \frac{C_{\mathrm{norm}}\mathrm{e}^{-\frac{(x-y)^2}{4k_{\mathrm{d}}t}}}{\sqrt{t}} \Theta\left(-\pi\zeta + \frac{\mathrm{i}\pi(x-y)}{2k_{\mathrm{d}}t}, \frac{\mathrm{i}\pi}{k_{\mathrm{d}}t}\right). \tag{12.25}$$

We may now rewrite the theta kernel in a more concise way, using that the theta function scales according to

$$\Theta(z,\tau) = (-\mathrm{i}\tau)^{-\frac{1}{2}} \exp\left(\frac{z^2}{\mathrm{i}\pi\tau}\right)\Theta\left(\frac{z}{\tau}, -\frac{1}{\tau}\right). \tag{12.26}$$

Choosing $\tau = \frac{\mathrm{i}\pi}{k_\mathrm{d} t}$ and $z = -\pi\zeta + \frac{\tau}{2}(x-y)$, we find

$$\Theta\left(-\pi\zeta + \frac{\mathrm{i}\pi(x-y)}{2k_\mathrm{d}t}, \frac{\mathrm{i}\pi}{k_\mathrm{d}t}\right) = \Theta\left(-\pi\zeta + \frac{\tau}{2}(x-y), \frac{\mathrm{i}\pi}{k_\mathrm{d}t}\right) = \Theta(z,\tau). \tag{12.27}$$

With $z^2/(\mathrm{i}\pi\tau) = -\zeta^2 k_\mathrm{d} t + \frac{(x-y)^2}{4k_\mathrm{d}t} + \mathrm{i}\zeta(x-y)$, we can then reformulate the Zak transform of ρ_t as

$$\begin{aligned}
\mathcal{Z}[\rho_t](x-y,\zeta) &= \frac{C_\mathrm{norm}}{\sqrt{t}}\frac{\sqrt{k_\mathrm{d}t}}{\sqrt{\pi}}\mathrm{e}^{-\zeta^2 k_\mathrm{d} t}\mathrm{e}^{\mathrm{i}\zeta(x-y)}\Theta\left(-\frac{\pi\zeta}{\tau} + \frac{1}{2}(x-y), -\frac{1}{\tau}\right)\\
&= C_\mathrm{norm}\frac{\sqrt{k_\mathrm{d}}}{\sqrt{\pi}}\mathrm{e}^{-\zeta^2 k_\mathrm{d} t}\mathrm{e}^{\mathrm{i}\zeta(x-y)}\Theta\left(\mathrm{i}\zeta k_\mathrm{d} t + \frac{1}{2}(x-y), -\frac{k_\mathrm{d}t}{\mathrm{i}\pi}\right)\\
&= \frac{C_\mathrm{norm}\sqrt{k_\mathrm{d}}}{\sqrt{\pi}}\sum_{n\in\mathbb{Z}}\mathrm{e}^{-(n+\zeta)^2 k_\mathrm{d} t}\mathrm{e}^{\mathrm{i}(n+\zeta)(x-y)},
\end{aligned} \tag{12.28}$$

using the very definition of the theta function during the last step.

We now have everything at hand that is needed to construct coherent states on the circle. Using again t for the classicality parameter and considering the analytic continuation of the image of the heat kernel, the not yet normalised coherent states on the circle read

$$\Psi^t_{\theta_0,p}(\phi;\zeta) = \left[\mathcal{Z}[\rho_t](\phi-y,\zeta)\right]_{y=\theta_0+\mathrm{i}p} \tag{12.29}$$

$$\begin{aligned}
&= \frac{C_\mathrm{norm}\sqrt{k_\mathrm{d}}}{\sqrt{\pi}}\mathrm{e}^{-\zeta^2 k_\mathrm{d} t}\mathrm{e}^{\mathrm{i}\zeta(\phi-(\theta_0+\mathrm{i}p))}\,\Theta\left(\mathrm{i}\zeta k_\mathrm{d} t + \frac{1}{2}(x-(\theta_0+\mathrm{i}p)), -\frac{k_\mathrm{d}t}{\mathrm{i}\pi}\right)\\
&= \frac{C_\mathrm{norm}\sqrt{k_\mathrm{d}}}{\sqrt{\pi}}\sum_{n\in\mathbb{Z}}\mathrm{e}^{-(n+\zeta)^2 k_\mathrm{d} t}\mathrm{e}^{\mathrm{i}(n+\zeta)\phi}\mathrm{e}^{-\mathrm{i}(n+\zeta)\theta_0}\mathrm{e}^{(n+\zeta)p}.
\end{aligned} \tag{12.30}$$

Therein, we used $\phi \in S^1$ for the coordinate, emphasising the states are defined on a circle for each fixed value of ζ — confer [206] for a proof. Note that we regain the U(1) complexifier coherent states of [208][2],

$$\Psi^t_{\theta_0,p}(\phi;\zeta) = \sum_{n=-\infty}^{\infty} \mathrm{e}^{-(n+\zeta)^2\frac{t}{2}}\mathrm{e}^{(n+\zeta)p}\mathrm{e}^{-\mathrm{i}(n+\zeta)\theta_0}\mathrm{e}^{\mathrm{i}(n+\zeta)\phi}, \tag{12.31}$$

if we choose $C_{\mathrm{norm}} = \sqrt{\frac{\pi}{k_{\mathrm{d}}}}$ and a diffusion constant of $k_{\mathrm{d}} = \frac{1}{2}$, leading to $C_{\mathrm{norm}} = \sqrt{2\pi}$. Comparing our result to the U(1) coherent states of [63, 64, 121, 133–135], we find different signs of θ_0 and ϕ for $\zeta = 0$. The origin of this discrepancy is their usage of the convention $\{p,q\} = 1$, leading to a complexified q of $z = q - \mathrm{i}p$. However, this is not problematic as the contribution of θ_0 is just a phase and concerning e.g. expectation values, the integral including ϕ is invariant under $\phi \mapsto -\phi$.

In what follows, we set $k_{\mathrm{d}} = \frac{1}{2}$ to be able to easier compare our results with the ones of [121, 133–135, 208]. ζ, however, will be kept arbitrary, allowing for a straightforward mapping between the U(1) scenario and the one of standard $L_2(\mathbb{R})$ via the Zak transformation at any time.

12.2 Semiclassical matrix elements

In this section, we first compute semiclassical expectation values with respect to coherent states on the circle of the dynamical operators discussed already in the quantum mechanical case during Section 11.3. We then continue with introducing a link between semiclassical matrix elements of $L_2(S^1)$ and $L_2(\mathbb{R})$ in Subsection 12.2.2.

12.2.1 Semiclassical expectation values via Kummer's functions

We use the previously constructed non-normalised U(1) coherent states on the circle in the form

$$\Psi^t_{\theta_0,p}(\phi;\zeta) = \sum_{n=-\infty}^{\infty} \mathrm{e}^{-\frac{t}{2}(n+\zeta)^2}\mathrm{e}^{\mathrm{i}(n+\zeta)(\phi-(\theta_0+\mathrm{i}p))} \tag{12.32}$$

[2] As stated above, the δ in [208] corresponds to our ζ.

and start with computing semiclassical expectation values of $|\hat{p}|^r$. The corresponding momentum operator of U(1) acts on these coherent states in the following way:

$$\hat{p}\Psi^t_{\theta_0,p}(\phi;\zeta) = -\mathrm{i}t\frac{\mathrm{d}}{\mathrm{d}\phi}\Psi^t_{\theta_0,p}(\phi;\zeta) = \sum_{n=-\infty}^{\infty}(n+\zeta)t\ \mathrm{e}^{-\frac{t}{2}(n+\zeta)^2}\mathrm{e}^{\mathrm{i}(n+\zeta)(\phi-(\theta_0+\mathrm{i}p))}. \tag{12.33}$$

The expectation value that we are interested in then reads

$$\langle\Psi^t_{\theta_0,p}(\zeta)\,|\,|\hat{p}|^r\,|\,\Psi^t_{\theta_0,p}(\zeta)\rangle = \left\|\Psi^t_{\theta_0,p}\right\|^{-2}\sum_{n\in\mathbb{Z}}|(n+\zeta)t|^r\mathrm{e}^{-t(n+\zeta)^2}\mathrm{e}^{2(n+\zeta)p}. \tag{12.34}$$

Compared to the usual case where ζ is fixed to be zero, we realise that the way the non-vanishing ζ enters into the expectation value is as a kind of shift of n. Therefore, if we apply the Poisson resummation formula now and use the modulation property of the Fourier transform, the result is the same as in the standard case up to an additional exponential of the form $\mathrm{e}^{2\mathrm{i}N\pi\zeta}$, where N denotes the summation index after the Poisson resummation has been performed. Thus, we obtain

$$\langle\Psi^t_{\theta_0,p}(\zeta)\,|\,|\hat{p}|^r\,|\,\Psi^t_{\theta_0,p}(\zeta)\rangle = \left\|\psi^t_g(\zeta)\right\|^{-2}\frac{\sqrt{2\pi}}{T}T^r\sum_{N=-\infty}^{\infty}\mathrm{e}^{2\mathrm{i}\pi N\zeta}\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{\sqrt{2\pi}}\,|x|^r\mathrm{e}^{-x^2+\frac{2p}{T}x-\frac{2\pi\mathrm{i}N}{T}x}, \tag{12.35}$$

where we defined $x := n+\zeta, T := \sqrt{t}$ and used the translation invariance of $\mathrm{d}x$. Now, we can proceed as in the quantum mechanical case. We rewrite $|x|^r$ in terms of the Kummer function of the second kind and afterwards write the integrand above as a product of the Fourier transform of the Kummer function, a Gaussian and a complex exponential. This yields

$$\begin{aligned}
&\langle\Psi^t_{\theta_0,p}(\zeta)\,|\,|\hat{p}|^r\,|\,\Psi^t_{\theta_0,p}(\zeta)\rangle\\
&= \left\|\psi^t_g(\zeta)\right\|^{-2}\frac{\sqrt{2\pi}}{T}T^r\sum_{N=-\infty}^{\infty}\mathrm{e}^{2\mathrm{i}\pi N\zeta}\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{\sqrt{2\pi}}\,U\Big(-\frac{r}{2},-\frac{r}{2}+1,x^2\Big)\mathrm{e}^{-x^2}\mathrm{e}^{\mathrm{i}x\left(\frac{-2\mathrm{i}p}{T}\right)}\mathrm{e}^{-\frac{2\pi\mathrm{i}N}{T}x}\\
&= \left\|\psi^t_g(\zeta)\right\|^{-2}\frac{\sqrt{2\pi}}{T}T^r\sum_{N=-\infty}^{\infty}\mathrm{e}^{2\mathrm{i}\pi N\zeta}\mathcal{F}\Big(U\Big(-\frac{r}{2},-\frac{r}{2}+1,x^2\Big)\mathrm{e}^{-x^2}\mathrm{e}^{\mathrm{i}x\left(\frac{-2\mathrm{i}p}{T}\right)}\Big)\left(\tfrac{2\pi N}{T}\right)\\
&= \left\|\psi^t_g(\zeta)\right\|^{-2}\frac{\sqrt{2\pi}}{T}T^r\frac{1}{\sqrt{2}}\frac{\Gamma\left(\frac{r+1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)}\sum_{N=-\infty}^{\infty}\mathrm{e}^{2\mathrm{i}\pi N\zeta}\mathrm{e}^{-\frac{\left(\frac{2\pi N}{T}+\frac{2\mathrm{i}p}{T}\right)^2}{4}}\,{}_1\mathrm{F}_1\left(-\frac{r}{2},\frac{1}{2},\frac{\left(\frac{2\pi N}{T}+\frac{2\mathrm{i}p}{T}\right)^2}{4}\right)
\end{aligned}$$

$$= \left\|\psi_g^t(\zeta)\right\|^{-2}\frac{T^r}{T}\Gamma\left(\tfrac{r+1}{2}\right)\sum_{N=-\infty}^{\infty}\mathrm{e}^{2\mathrm{i}\pi N\zeta}\mathrm{e}^{-\frac{(\pi N+\mathrm{i}p)^2}{T^2}}{}_1\mathrm{F}_1\left(-\frac{r}{2},\frac{1}{2},\left(\frac{\pi N}{T}+\frac{\mathrm{i}p}{T}\right)^2\right), \tag{12.36}$$

where we applied Lemma 1 in the second step and also used $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$. Using the Kummer transformation for ${}_1\mathrm{F}_1(a, b, z)$ shown in (11.11), we finally obtain

$$\begin{aligned}&\langle\Psi^t_{\theta_0,p}(\zeta)\,|\,|\hat{p}|^r\,|\,\Psi^t_{\theta_0,p}(\zeta)\rangle\\ &\quad= \left\|\psi_g^t(\zeta)\right\|^{-2}\frac{T^r}{T}\Gamma\left(\tfrac{r+1}{2}\right)\sum_{N=-\infty}^{\infty}\mathrm{e}^{2\mathrm{i}\pi N\zeta}{}_1\mathrm{F}_1\left(\frac{r+1}{2},\frac{1}{2},\left(\frac{p-\pi\mathrm{i}N}{T}\right)^2\right).\end{aligned} \tag{12.37}$$

To complete this calculation, let us compute the norm of the coherent states that is involved in the result above. After the Poisson resummation, we get

$$\left\|\psi_g^t(\zeta)\right\|^2 = \sum_{n=-\infty}^{\infty}\mathrm{e}^{-t(n+\zeta)^2}\mathrm{e}^{2(n+\zeta)p} = \sqrt{\frac{\pi}{T^2}}\sum_{N=-\infty}^{\infty}\mathrm{e}^{2\pi\mathrm{i}N\zeta}\ \mathrm{e}^{-\frac{(\mathrm{i}\pi p+N\pi)^2}{T^2}}. \tag{12.38}$$

Being now interested in the asymptotics of small t, and hence T accordingly, we can apply the asymptotic expansion for large arguments of the KCHF, (11.18), on (12.37). This follows closely the procedure of the quantum mechanical scenario of (11.30). With the norm (12.38), a Gaussian in p^2/t enters the expectation value. Hence, out of the two series of the KCHF's asymptotic expansion, only the one with the inverse Gaussian in p^2/t remains, while the other one is damped to $\mathcal{O}(t^\infty)$. In the end, we obtain

$$\begin{aligned}\langle\Psi^t_{\theta_0,p}(\zeta)\,|\,|\hat{p}|^r\,|\,\Psi^t_{\theta_0,p}(\zeta)\rangle &= |p|^r\sum_{n=0}^{\infty}\frac{\left(-\frac{r}{2}\right)_n\left(\frac{1-r}{2}\right)_n}{n!}\left(\frac{t}{p^2}\right)^n\\ &= |p|^r\left(1-\frac{r(1-r)}{4}\frac{t}{p^2}+\mathcal{O}\left(t^2\right)\right),\end{aligned} \tag{12.39}$$

which resembles perfectly the quantum mechanical result of (11.30). That this is expected will be discussed in detail in Subsection 12.2.2, where the relation between semiclassical expectation values of quantum mechanics and U(1) is analysed by means of the Zak transform and its properties.

Before this, we now compute semiclassical expectation values of the class of operators $\hat{q}(r)$, which as already stated are of great importance in loop quantum gravity. With the previously obtained results of (12.37) and (12.38), we may now also rigorously compute expectation values of them in U(1). From (12.37), we can directly derive the expectation value of $|\hat{p}|^r$ w.r.t. the coherent state the inverse holonomy acted on:

$$\begin{aligned}&\langle \hat{h}^{-1}\Psi^t_{\theta_0,p}(\zeta)\,|\,|\hat{p}|^r\,|\,\hat{h}^{-1}\Psi^t_{\theta_0,p}(\zeta)\rangle\\&=\left\|\psi^t_g(\zeta)\right\|^{-2}\frac{T^r}{T}\Gamma\left(\tfrac{r+1}{2}\right)\sum_{N=-\infty}^{\infty}\mathrm{e}^{2\mathrm{i}\pi N\zeta}{}_1\mathrm{F}_1\left(\frac{r+1}{2},\frac{1}{2},\left(\frac{p-T^2-\pi\mathrm{i}N}{T}\right)^2\right).\end{aligned}\tag{12.40}$$

Like in the standard quantum mechanical case of Section 11.3, the inverse holonomy acting on the coherent state causes an (infinitesimal) shift in the momentum. With the holonomy being $h=\mathrm{e}^{\mathrm{i}\phi}$, the momentum operator's ϕ-derivative now not only sees $\mathrm{e}^{-\mathrm{i}(n+\zeta)\phi}$ as in (12.33), but acts on $\mathrm{e}^{\mathrm{i}(n+\zeta)\phi}\mathrm{e}^{-\mathrm{i}\phi}=\mathrm{e}^{\mathrm{i}(n+\zeta-1)\phi}$ instead. Hence, $|\hat{p}|^r$ acting on the shifted coherent state evaluates now $|(n+\zeta-1)t|^r$ and we can cast that shift into $p\mapsto p-t$ in the state's exponentials via a redefinition of $n\mapsto n-1$. Having these two expectation values of $|\hat{p}|^r$, we can combine them to the commutator's expectation value and proceed as before in the quantum mechanical case, namely by performing the asymptotic expansion for large arguments of the KCHFs, as both of them grow with $\frac{1}{t}$ for small t. In the end, we obtain

$$\langle \hat{q}^r\rangle_{\Psi^t_{\theta_0,p}}\approx\frac{r|p|^r}{p}t+|p|^r\left(\frac{r(1-r)}{2p^2}+\frac{r(2-3r+r^2)}{4p^3}\right)t^2+\mathcal{O}(t^3).\tag{12.41}$$

We see again that the series' first term corresponds one-to-one to the derivative's result. For the next order, we got two contributions: one that resembles the second derivative but also a further one. If we compare the result above to the quantum mechanic's result of (11.35), we notice that the $\hbar^2$-contribution there also comprised two terms. While one included α^2, namely the one with the numerical prefactors and powers of p in accordance to the second derivative, the second one was proportional to α.

12.2.2 Linking semiclassical matrix elements of $L_2(S^1)$ and $L_2(\mathbb{R})$

As discussed in Section 12.1, the Zak transformation provides a unitary map between the Hilbert spaces $L_2(\mathbb{R})$ and $L_2(\mathbb{R}^2/\mathbb{Z}^2)$. Therefore, the expectation values of the usual quantum mechanical operators and their corresponding Zak-transformed counterparts are identical. However, if we compute matrix elements or semiclassical expectation values with respect to U(1) coherent states for fixed ζ, as one does for coherent states on a circle, we only perform one of the integrals, namely the one over θ, out of the two integrations involved in the inner product of $L_2(\mathbb{R}^2/\mathbb{Z}^2)$. Nevertheless, as we will show below, the expectation value with respect to U(1) coherent states is completely determined if we know the matrix elements of the corresponding operator with respect to the harmonic oscillator coherent states in $L_2(\mathbb{R})$. As shown above, the U(1) coherent states can be written by means of the Zak transform as $\psi_g^t(\phi,\zeta) = \mathcal{Z}[\Psi^\hbar_{q,p}](\phi,\zeta)$, and accordingly operators $\hat{O}_{\mathrm{QM}}$ transform under $\mathcal{Z}$ as $\mathcal{Z}\hat{O}_{\mathrm{QM}}\mathcal{Z}^{-1}$. Hence, the integrand of an $L_2(S^1)$ expectation value with respect to U(1) coherent states is given by

$$\overline{\mathcal{Z}[\Psi^\hbar_{q,p}]}(\phi,\zeta)\mathcal{Z}\hat{O}_{\mathrm{QM}}\mathcal{Z}^{-1}\mathcal{Z}[\Psi^\hbar_{q,p}](\phi,\zeta) = \overline{\mathcal{Z}[\Psi^\hbar_{q,p}]}(\phi,\zeta)\mathcal{Z}[\hat{O}_{\mathrm{QM}}\Psi^\hbar_{q,p}](\phi,\zeta). \tag{12.42}$$

In the following considerations, we want to examine the relation between

$$\int_0^{2\pi}\frac{\mathrm{d}\phi}{2\pi}\overline{\mathcal{Z}[\Psi^\hbar_{q,p}]}(\phi,\zeta)\mathcal{Z}[\hat{O}_{\mathrm{QM}}\Psi^\hbar_{q,p}](\phi,\zeta)$$

and matrix elements $\langle\Psi^\hbar_{q',p'}\,|\,\hat{O}_{\mathrm{QM}}\,|\,\Psi^\hbar_{q,p}\rangle_{L_2(\mathbb{R})}$. We will follow [231], where some of the formulae are presented but partly without proofs[3]. With $f,g\in L_2(R)$, $\overline{\mathcal{Z}[f]}(\phi,\zeta)\mathcal{Z}[g](\phi,\zeta)$ is periodic in ζ, which follows directly from the definition of the Zak transform. Furthermore, it is also 2π-periodic in ϕ: We have

$$\overline{\mathcal{Z}[f]}(\phi+2\pi,\zeta)\mathcal{Z}[g](\phi+2\pi,\zeta) = \sum_{m,n=-\infty}^{\infty}\overline{f}(\phi+2\pi+2\pi m)\;\mathrm{e}^{\mathrm{i}2\pi m\zeta}g(\phi+2\pi+2\pi n)\;\mathrm{e}^{-\mathrm{i}2\pi n\zeta} \tag{12.43}$$

$$\overset{\substack{r:=m+1\\ s:=n+1}}{=}\sum_{r,s=-\infty}^{\infty}\overline{f}(\phi+2\pi r)\;\mathrm{e}^{\mathrm{i}2\pi(r-1)\zeta}g(\phi+2\pi s)\;\mathrm{e}^{-\mathrm{i}2\pi(s-1)\zeta} \tag{12.44}$$

$$= \sum_{r,s=-\infty}^{\infty}\overline{f}(\phi+2\pi r)\;\mathrm{e}^{\mathrm{i}2\pi r\zeta}g(\phi+2\pi s)\;\mathrm{e}^{-\mathrm{i}2\pi s\zeta} \tag{12.45}$$

$$= \overline{\mathcal{Z}[f]}(\phi,\zeta)\,\mathcal{Z}[g](\phi,\zeta). \tag{12.46}$$

As a consequence, we can expand $\mathcal{Z}[f]\mathcal{Z}[g]$ into a Fourier series given by

$$(\overline{\mathcal{Z}[f]}\mathcal{Z}[g])(\phi,\zeta) = \sum_{m,n=-\infty}^{\infty}\mathcal{F}_{mn}\;\mathrm{e}^{\mathrm{i}xm}\;\mathrm{e}^{2\pi\mathrm{i}n\zeta}, \tag{12.47}$$

[3]Note that in [231], some definitions might differ by factors of π because we adopted the operators to the case needed for our work.

where $\mathcal{F}_{mn}$ denote the Fourier coefficients that have the form

$$\mathcal{F}_{mn} = \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^1 d\zeta \Big(\overline{\mathcal{Z}[f]}\mathcal{Z}[g]\Big)(\phi,\zeta)\ e^{-imx}\ e^{-2\pi in\zeta}. \tag{12.48}$$

Next, we introduce the translation and scaling operators defined by

$$(T_a f)(x) := f(x+a) \quad \text{and} \quad (R_b f)(x) := e^{-ibx} f(x), \quad a,b \in \mathbb{R}. \tag{12.49}$$

The Fourier coefficients $\mathcal{F}_{mn}$ can be easily computed as already discussed in [231] and in more detail in [232]:

Lemma 2 *The Fourier coefficients $\mathcal{F}_{mn}$ in*

$$(\overline{\mathcal{Z}[f]}\mathcal{Z}[g])(\phi,\zeta) = \sum_{m,n=-\infty}^{\infty} \mathcal{F}_{mn}\ e^{ixm}\ e^{2\pi in\zeta} \tag{12.50}$$

are given by

$$\mathcal{F}_{mn} = \langle R_{-m} T_{2\pi n} f\, ,\, g\rangle_{L_2(\mathbb{R})}. \tag{12.51}$$

In order to proof the lemma above, we just have to compute the Zak transform of $R_{-m}T_{2\pi n}f$. We obtain

$$\begin{aligned}
\mathcal{Z}[R_{-m}T_{2\pi n}f](\phi,\zeta) &= \sum_{k=-\infty}^{\infty} (R_{-m}T_{2\pi n}f)(\phi+2\pi k)\ e^{-2i\pi k\zeta} \\
&= \sum_{k=-\infty}^{\infty} f(\phi+2\pi(k+n))\ e^{-2i\pi k\zeta}\ e^{i(\phi+2\pi(k+n))m} \\
&= \sum_{k=-\infty}^{\infty} f(\phi+2\pi k)\ e^{2i\pi n\zeta}\ e^{-2i\pi k\zeta}\ e^{i\phi m} \\
&= \mathcal{Z}[f](\phi,\zeta)\ e^{i\phi m}\ e^{2\pi i\zeta n},
\end{aligned} \tag{12.52}$$

where we used the quasi-periodicity of $\mathcal{Z}$ in the second last step. Given this, the complex conjugate reads

$$\overline{\mathcal{Z}[R_{-m}T_{2\pi n}f]}(\phi,\zeta) = \overline{\mathcal{Z}[f]}(\phi,\zeta)e^{-i\phi m}e^{-2\pi i\zeta n}. \tag{12.53}$$

Reinserting this back into the Fourier coefficients $\mathcal{F}_{mn}$, we get

$$\begin{aligned}\mathcal{F}_{mn} &= \int_0^{2\pi} \frac{\mathrm{d}\phi}{2\pi} \int_0^1 \mathrm{d}\zeta \overline{\mathcal{Z}[R_{-m}T_{2\pi n}f]}\mathcal{Z}[g](\phi,\zeta) \\ &= \langle \overline{\mathcal{Z}[R_{-m}T_{2\pi n}f]}\,,\, \mathcal{Z}[g]\rangle_{L_2(S^1\times(S^1)^*)} \\ &= \langle R_{-m}T_{2\pi n}f\,,\, g\rangle_{L_2(\mathbb{R})}, \end{aligned} \tag{12.54}$$

where we used the unitarity of the Zak transform in the last step. Therefore, the Fourier series associated with $\langle \overline{\mathcal{Z}}[f](\zeta)\,,\, \mathcal{Z}[g](\zeta)\rangle_{L_2(S^1)}$ reads

$$\begin{aligned}\langle \overline{\mathcal{Z}}[f](\zeta)\,,\, \mathcal{Z}[g](\zeta)\rangle_{L_2(S^1)} &= \int_0^{2\pi} \frac{\mathrm{d}\phi}{2\pi} \sum_{m,n=-\infty}^{\infty} \langle R_{-m}T_{2\pi n}f\,,\, g\rangle_{L_2(\mathbb{R})}\, \mathrm{e}^{\mathrm{i}m\phi}\, \mathrm{e}^{2\mathrm{i}\pi n\zeta} \\ &= \sum_{n=-\infty}^{\infty} \langle T_{2\pi n}f\,,\, g\rangle_{L_2(\mathbb{R})}\, \mathrm{e}^{2\mathrm{i}\pi n\zeta}. \end{aligned} \tag{12.55}$$

If we apply the result in (12.55) on the harmonic oscillator coherent states, we obtain the following relation between semiclassical matrix elements in $L_2(S^1)$ and $L_2(\mathbb{R})$:

Lemma 3 *For a linear operator $\hat{O}$ on (a suitable domain of) $L_2(S^1)$ that is obtained from the corresponding operator $\hat{O}_{\mathrm{QM}}$ on (a suitable domain of) $L_2(\mathbb{R})$ by $\hat{O} = \mathcal{Z}\hat{O}_{\mathrm{QM}}\mathcal{Z}^{-1}$ we have the following relation between the matrix elements in $L_2(S^1)$ and $L_2(\mathbb{R})$:*

$$\langle \Psi^t_{\theta_0',p'}(\zeta)\,|\,\hat{O}\,|\,\Psi^t_{\theta_0,p}(\zeta)\rangle_{L_2(S^1)} = \sum_{n=-\infty}^{\infty} \mathrm{e}^{2\mathrm{i}\pi n\zeta}\langle T_{2\pi n}\Psi^{\hbar}_{q',p'}\,|\,\hat{O}_{\mathrm{QM}}\,|\Psi^{\hbar}_{q,p}\rangle_{L_2(\mathbb{R})}\Big|_{\substack{t=\hbar \\ \theta_0=q \bmod 2\pi \\ \theta_0'=q' \bmod 2\pi}}. \tag{12.56}$$

We realise the semiclassical matrix elements in $L_2(S^1)$ can be understood as a Fourier series in ζ with Fourier coefficients $c_n := \langle T_{2\pi n}f, g\rangle_{L_2(\mathbb{R})}$. This means that the matrix elements in $L_2(S^1)$ are completely determined by the corresponding matrix elements in the ordinary quantum mechanics case in $L_2(\mathbb{R})$. In particular, an additional integration over $\int_0^1 d\zeta$ just projects onto the $n = 0$ coefficient and this yields, as expected from the unitarity of $\mathcal{Z}$, the semiclassical matrix element in $L_2(\mathbb{R})$.

Expectation values of U(1) coherent states for integer powers of holonomy and momentum operators have been computed in [134, 135, 208] using complexifier coherent states. In [134, 135], these were computed for the special case of $\zeta = 0$, whereas in [208] an arbitrary ζ was considered. In both works, they show that it is justified to only consider the $n=0$ term if we are interested in the classical limit $t \to 0$. Given this, we know from the lemma above that in this limit the result for $L_2(S^1)$ and $L_2(\mathbb{R})$ exactly coincide and the value of ζ is irrelevant. In [205–207], these kind of expectation values were computed and higher n terms were rewritten in terms of Jacobi's theta function and its derivative respectively. We believe that the relation shown in the lemma above yields a simpler formulation of the higher order terms in n and easily allows to extract the semiclassical limit $t \to 0$.

To demonstrate that Lemma 3 may indeed simplify computations of semiclassical matrix elements and expectations values, we apply it to a couple of examples. First, we consider the overlap of two coherent states and thus choose $f = \Psi^{\hbar}_{q',p'}$ and $g = \Psi^{\hbar}_{q,p}$. The matrix element of interest in $L_2(\mathbb{R})$ is then

$$\langle T_{2\pi n}\Psi^{\hbar}_{q',p'}\,|\Psi^{\hbar}_{q,p}\rangle_{L_2(\mathbb{R})} = \sqrt{\frac{\pi}{\hbar}}\;\mathrm{e}^{-\frac{1}{\hbar}\left(\frac{q-q'+\mathrm{i}(p+p')}{2}+n\pi\right)^2}. \tag{12.57}$$

Given this, the corresponding overlap for $L_2(S^1)$ reads

$$\langle \Psi^{t}_{\theta_0',p'}(\zeta)\,|\,\Psi^{t}_{\theta_0,p}(\zeta)\rangle_{L_2(S^1)} = \sqrt{\frac{\pi}{t}}\sum_{n=-\infty}^{\infty}\mathrm{e}^{-\frac{1}{\hbar}\left(\frac{q-q'+\mathrm{i}(p+p')}{2}+n\pi\right)^2}\mathrm{e}^{2\pi\mathrm{i}n\zeta}\;\Big|_{\substack{t=\hbar\\ \theta_0=q \bmod 2\pi\\ \theta_0'=q' \bmod 2\pi}}, \tag{12.58}$$

which exactly agrees with the result in [208] and reproduces also the correct result for the norm, for instance computed in [133, 135, 208], as a special case:

$$\langle \Psi^{t}_{\theta_0,p}(\zeta)\,|\,\Psi^{t}_{\theta_0,p}(\zeta)\rangle_{L_2(S^1)} = \left\|\Psi^{t}_{\theta_0,p}\right\|^2 = \sqrt{\frac{\pi}{t}}\sum_{n=-\infty}^{\infty}\mathrm{e}^{-\frac{1}{t}(\mathrm{i}p+n\pi)^2}\mathrm{e}^{2\pi\mathrm{i}n\zeta}. \tag{12.59}$$

In our further discussion, we will consider semiclassical expectation values of the basic operators as well as matrix elements for fractional powers of the momentum operator. We start with integer powers of holonomy operators, that is $\hat{h}^m = \mathrm{e}^{\mathrm{i}m\hat{x}}$. For this operator, we get

$$\langle T_{2\pi n}\Psi^{\hbar}_{q,p}\,|\,\mathrm{e}^{\mathrm{i}m\hat{x}}\,|\,\Psi^{\hbar}_{q,p}\rangle_{L_2(\mathbb{R})} = \sqrt{\frac{\pi}{\hbar}}\;\mathrm{e}^{-\frac{1}{\hbar}(\mathrm{i}p+n\pi)^2}\mathrm{e}^{\mathrm{i}m(q-\frac{m\hbar}{4})}\mathrm{e}^{-\mathrm{i}\pi nm}, \tag{12.60}$$

and therefore the corresponding semiclassical expectation value for U(1) coherent states yields

$$\langle \Psi^t_{\theta_0,p}(\zeta) \,|\, \mathrm{e}^{\mathrm{i}m\hat{\phi}} \,|\, \Psi^t_{\theta_0,p}(\zeta) \rangle_{L_2(S^1)} = \sqrt{\frac{\pi}{t}}\ \mathrm{e}^{\mathrm{i}m(q-\frac{mt}{4})} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-\frac{1}{t}(\mathrm{i}p+n\pi)^2} \mathrm{e}^{-\mathrm{i}\pi nm} \mathrm{e}^{2\pi\mathrm{i}n\zeta} \,\Big|_{\substack{t=\hbar \\ \theta_0=q \bmod 2\pi \\ \theta_0'=q' \bmod 2\pi}},$$

which agrees for $m = 1$ and up to a different normalisation with the results in [205, 207]. We cannot directly compare it to the results in [135], since they only considered the limit $t \to 0$ and thus some terms were neglected during the computation.

Let us briefly discuss the matrix elements in $L_2(\mathbb{R})$ that enter the Fourier expansion of semiclassical expectation values in $L_2(S^1)$. For an operator of the form $\hat{O} = f(\hat{x})$, the Fourier coefficients have the following form:

$$\langle T_{2\pi n} \Psi^\hbar_{q,p} \,|\, f(\hat{x}) \,|\, \Psi^\hbar_{q,p} \rangle_{L_2(\mathbb{R})} = \frac{1}{\hbar}\ \mathrm{e}^{-\frac{1}{t}(\mathrm{i}p+n\pi)^2} \int_{\mathbb{R}} \mathrm{d}x f(x)\ \mathrm{e}^{-\frac{1}{\hbar}(x-q+\pi n)^2}.$$

We realise that the only difference to the case $n = 0$, when the translation operator becomes the identity operator, is that (some) q and p labels get shifted by $n\pi$ or $-n\pi$ respectively. Note that this cannot be carried over to a shift in the q, p labels for the entire state $\Psi^\hbar_{q,p}$ since also the normalisation constant $C_{q,p,\hbar}$ depends on these labels and no shift occurs there. Likewise, considering the Fourier transform of the states $\Psi^\hbar_{q,p}$, we can write down a smilar result for operators $\hat{O} = f(\hat{p})$ given by

$$\langle T_{2\pi n} \Psi^\hbar_{q,p} \,|\, f(\hat{p}) \,|\, \Psi^\hbar_{q,p} \rangle_{L_2(\mathbb{R})} = \frac{1}{\hbar} \int_{\mathbb{R}} \mathrm{d}k\ \mathrm{e}^{-\frac{1}{\hbar}k^2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}k(-\mathrm{i}p+n\pi)} f(k).$$

Now, if we choose as an example $f(\hat{p}) = |\hat{p}|^r$, we can easily show that the result in (12.37) is consistent with Lemma 3. This also explains the additional shift by $n\pi$ in the argument of the Kummer function compared to the result for the quantum mechanical expectation value of (11.29), yielding a consistency check of our computations in the former sections. Moreover, for $n = 0$ the results of (12.36) and (11.29) agree as required if the normalisation is taken correctly.

Finally, we present the computation of matrix elements for fractional powers of the momentum operator, that is we are aiming at computing $\langle \Psi^t_{\theta_0',p'}(\zeta) \,|\, |\hat{p}|^r \,|\, \psi^t_g(\zeta) \rangle_{L_2(S^1)}$ by applying Lemma 3. For this purpose we need the explicit form of

$$\langle T_{2\pi n}\Psi^{\hbar}_{q'p'} \,|\, |\hat{p}|^r \,|\, \Psi^{\hbar}_{q,p}\rangle_{L_2(\mathbb{R})} = \int \mathrm{d}k\, \mathcal{F}(\overline{\Psi^{\hbar}_{q'p'}})(k)|k|^r \mathcal{F}(\Psi^{\hbar}_{q,p})(k) e^{-\frac{\mathrm{i}}{\hbar}2\pi nk}. \tag{12.61}$$

Reinserting the Fourier transform $\mathcal{F}(\Psi^{\hbar}_{q,p})(k) = C_{q,p,\hbar}e^{-\frac{1}{2\hbar}(k-p)^2}e^{-\frac{\mathrm{i}}{\hbar}(k-p)q}$ together with $C_{q,p,\hbar}e^{-\frac{1}{2\hbar}p^2+\frac{\mathrm{i}}{\hbar}pq} = \frac{1}{\sqrt{\hbar}}$ and $\overline{C}_{q',p',\hbar}e^{-\frac{1}{2\hbar}(p')^2-\frac{\mathrm{i}}{\hbar}p'q'} = \frac{1}{\sqrt{\hbar}}$, we obtain

$$\langle T_{2\pi n}\Psi^{\hbar}_{q'p'} \,|\, |\hat{p}|^r \,|\, \Psi^{\hbar}_{q,p}\rangle_{L_2(\mathbb{R})} = \hbar^{\frac{r}{2}-1}\int \mathrm{d}k \left|\frac{k}{\sqrt{\hbar}}\right|^r e^{-\frac{1}{\hbar}k^2} e^{\frac{\mathrm{i}}{\sqrt{\hbar}}k\left(\frac{q'-\mathrm{i}p'}{\sqrt{\hbar}}-\frac{q+\mathrm{i}p}{\sqrt{\hbar}}-\frac{2\pi n}{\sqrt{\hbar}}\right)}. \tag{12.62}$$

Next, we rewrite the absolute value in terms of the Kummer function of the first kind, that is $\left|\frac{k}{\sqrt{\hbar}}\right|^r = U(-\frac{r}{2}, -\frac{r}{2}+1, \frac{k^2}{\hbar})$. Further, we introduce the new variable $\tilde{k} := \frac{k}{\sqrt{\hbar}}$ and perform the integration by using the duality of Kummer's function of the first and second kind under Fourier transformations, as discussed in Section 11.1. This yields

$$\begin{aligned}\langle T_{2\pi n}\Psi^{\hbar}_{q'p'} \,|\, |\hat{p}|^r \,|\, \Psi^{\hbar}_{q,p}\rangle_{L_2(\mathbb{R})} &= \\ &= \sqrt{\frac{\pi}{\hbar}}\frac{\Gamma(\frac{r+1}{2})}{\Gamma(\frac{1}{2})}\hbar^{\frac{r}{2}} e^{-\frac{1}{\hbar}\left(\frac{q-q'+\mathrm{i}(p+p')}{2}+n\pi\right)^2} {}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, \frac{1}{\hbar}\left(\frac{q-q'+\mathrm{i}(p+p')}{2}+n\pi\right)^2\right).\end{aligned} \tag{12.63}$$

If we specialise the above result to the case $r = 0$ and consider that ${}_1\mathrm{F}_1\big(0, \frac{1}{2}, z\big) = 1$ for all z, then the result exactly agrees with the overlap shown in (12.57). Given the result for the matrix element in $L_2(\mathbb{R})$ by means of Lemma 3, we immediately get the analogue for $L_2(S^1)$, which finally takes the form

$$\begin{aligned}\langle \Psi^t_{\theta_0',p'}(\zeta) \,|\, |\hat{p}|^r \,|\, \Psi^t_{\theta_0,p}(\zeta)\rangle_{L_2(S^1)} &= \\ &= \sqrt{\frac{\pi}{t}}\frac{\Gamma(\frac{r+1}{2})}{\Gamma(\frac{1}{2})}t^{\frac{r}{2}}\sum_{n=0}^{\infty} e^{\mathrm{i}2\pi n\zeta} e^{-\frac{1}{t}\left(\frac{q-q'+i(p+p')}{2}+n\pi\right)^2} {}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, \frac{1}{t}\left(\frac{q-q'+\mathrm{i}(p+p')}{2}+n\pi\right)^2\right) \Big|_{\substack{t=\hbar \\ \theta_0=q \bmod 2\pi \\ \theta_0'=q' \bmod 2\pi}}.\end{aligned} \tag{12.64}$$

Comparing the final result in (12.64) to the result in (12.36), we realise that if we choose $\theta_0' = \theta_0$ and $p' = p$ corresponding to $q' = q$ and $p' = p$ in (12.64) as well as take into account that $T = \sqrt{t}$, then for this special case the results in (12.36) and (12.64) exactly coincide. As can be seen for all examples discussed in this subsection, Lemma 3 provides a method to compute semiclassical matrix elements for $L_2(S^1)$ by computing the corresponding shifted matrix elements in $L_2(\mathbb{R})$. In the next section, we will discuss the relation between the Zak transform and the Poisson resummation formula.

12.3 The Zak transformation and the Poisson resummation formula

In the framework of complexifier coherent states, the Poisson resummation formula is heavily used during computations of semiclassical matrix elements. For the benefit of the reader, we therefore review the relation between the Zak transformation and the Poisson resummation by following [233]. In order to relate the Zak transformation to the Poisson resummation formula, we introduces a dual Zak transformation $\widetilde{\mathcal{Z}}$ defined as

$$\widetilde{\mathcal{Z}}[f](x,\zeta) = \sum_{n=-\infty}^{\infty} f(\zeta+n)\, \mathrm{e}^{\mathrm{i}nx}.$$

For $g(x,\zeta) = \mathcal{Z}[f](x,\zeta)$ and $\tilde{g}(x,\zeta) = \widetilde{\mathcal{Z}}[f](x,\zeta)$, the inverse of $\mathcal{Z}$ and $\widetilde{\mathcal{Z}}$ are given by

$$\mathcal{Z}^{-1}[g](x) = \int_0^1 \mathrm{d}\zeta g(x,\zeta) \quad \text{and} \quad \widetilde{\mathcal{Z}}^{-1}[\tilde{g}](\zeta) = \int_0^{2\pi} \frac{\mathrm{d}x}{2\pi} \tilde{g}(x,\zeta).$$

Defining the operator $\mathcal{U}[g](x,\zeta) := \mathrm{e}^{-\mathrm{i}x\zeta} g(x,\zeta)$, it is easy to show that $\widetilde{\mathcal{Z}}^{-1}\mathcal{U}\mathcal{Z}[f] = \sqrt{2\pi}\mathcal{F}[f]$ and hence related to the Fourier transformation. Likewise, one can also show that $\mathcal{Z}^{-1}\mathcal{U}^{-1}\widetilde{\mathcal{Z}} = \sqrt{2\pi}\mathcal{F}^{-1}(f)$. We just consider the case of the Fourier transform here, for which we have

$$\begin{aligned}
\widetilde{\mathcal{Z}}^{-1}\mathcal{U}\mathcal{Z}[f] &= \int_0^{2\pi} \frac{\mathrm{d}x}{2\pi} \sum_{k=-\infty}^{\infty} f(x+2\pi k)\, \mathrm{e}^{-2\mathrm{i}\pi k\zeta}\, \mathrm{e}^{-\mathrm{i}x\zeta} \\
&= \sum_{k=-\infty}^{\infty} \int_0^{2\pi} \frac{\mathrm{d}x}{2\pi} f(x+2\pi k)\, \mathrm{e}^{-\mathrm{i}(x+2\pi k)\zeta} \\
&= \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}x f(x)\, \mathrm{e}^{-\mathrm{i}x\zeta} = \sqrt{2\pi}\mathcal{F}[f](\zeta).
\end{aligned} \tag{12.65}$$

With this, we equivalently have

$$\mathcal{U}\mathcal{Z}[f] = \sqrt{2\pi}\widetilde{Z}[\mathcal{F}[f]]. \tag{12.66}$$

Considering the explicit forms of $\mathcal{Z}$ and $\widetilde{\mathcal{Z}}$, we finally obtain

$$\sum_{n=-\infty}^{\infty} f(x+2\pi n)\, \mathrm{e}^{-2\pi\mathrm{i}n\zeta}\, \mathrm{e}^{-\mathrm{i}x\zeta} = \sqrt{2\pi} \sum_{n=-\infty}^{\infty} \mathcal{F}[f](\zeta+n)\, \mathrm{e}^{\mathrm{i}nx}. \tag{12.67}$$

If we now choose $\zeta = x = 0$, we obtain the standard Poisson resummation formula. As far as the application on complexifier coherent states is considered, we can choose $f := g \circ S_t$, where S_t is a scaling by the classicality parameter t defined as $S_t x := \frac{x}{\sqrt{t}}$, and we obtain the form of the Poisson resummation formula used in this context.

12.4 Kummer's functions and the heat equation

In this section, we briefly discuss the physical interpretation of Kummer functions in the context of self-similar solutions of the heat equation following closely the ideas of [212] and slightly generalising some aspects of their work. We start with the heat equation

$$\frac{\partial u}{\partial t}(x,t) = k_{\mathrm{d}} \frac{\partial^2}{\partial x^2} u(x,t). \tag{12.68}$$

Along the lines of [212], we introduce self-similar coordinates (ξ, τ) given by

$$\tau := \tau(t) \quad \text{and} \quad \xi := \frac{x}{\sqrt{k_{\mathrm{d}}} L(\tau)}, \tag{12.69}$$

where the explicit form of the functions L and τ still needs to be determined. As an ansatz for a self-similar solution of the heat equation, we consider

$$u(x,t) = A(\tau(t)) w(\xi(x,t), \tau(t)), \tag{12.70}$$

which leads to the following differential equation:

$$\dot{\tau} \left(\left(\frac{A'}{A} \right) w + \frac{\partial w}{\partial \tau} - \left(\frac{L'}{L} \right) \frac{\partial w}{\partial \xi} \right) = \frac{k_{\mathrm{d}}}{k_{\mathrm{d}} L^2(\tau)} \frac{\partial^2}{\partial \xi^2} w, \tag{12.71}$$

where the dot denotes a derivative with respect to t and a prime one with respect to τ. Now, the requirements made in [212] are that the self-similar solution is static in the (ξ, τ)-frame, and hence there cannot be any explicit time-dependence. This yields a relation between τ and $L(\tau)$ of the form $\dot{\tau} \overset{!}{=} \frac{1}{L^2(\tau)}$. Furthermore, we are only interested in solutions for which $\frac{L'}{L} =: G = \text{const} > 0$ and $\frac{A'}{A} =: \beta = \text{const}$.[4] As can be seen directly from (12.71), the first condition corresponds to a constant expansion rate and the second condition determines the scaling of the amplitude $A(\tau(t))$ with t parametrised by b. As

[4] Note that our β is equal to b in the notation of [212].

shown in [212], these conditions yield the following expressions for the functions L and A:

$$\begin{aligned} L(\tau) &= L_0 \mathrm{e}^{G\tau} \quad \Leftrightarrow \quad L(t) = \sqrt{2G}(t-t_0)^{\frac{1}{2}} \quad \text{and} \\ A(\tau) &= A_0 \mathrm{e}^{\beta\tau} \quad \Leftrightarrow \quad A(t) = A_0 \left(\frac{2G}{L_0^2}(t-t_0)\right)^{\frac{\beta}{2G}}. \end{aligned} \tag{12.72}$$

We realise that the scaling of $L(t)$ is always with $t^{1/2}$, whereas the one of $A(t)$ can be different from $t^{-1/2}$, which holds for the heat kernel solution, for appropriate choices of $\frac{\beta}{G}$ — as emphasised by the authors in [212]. With the above assumptions at hand, the differential equation that w has to satisfy for a static self-similar solution of the heat equation in the (ξ, τ)-frame reads

$$\frac{\partial^2}{\partial \xi^2} w + G\xi \frac{\partial}{\partial \xi} w - \beta w = 0. \tag{12.73}$$

Introducing the following scaling of the ξ-coordinate as well as the variable W

$$\tilde{\xi} := \sqrt{\frac{G}{2}}\xi, \qquad W := \mathrm{e}^{\frac{\tilde{\xi}^2}{2}} w, \tag{12.74}$$

the differential equation for w in (12.73) can be transformed into a generalised Hermite differential equation for W given by

$$\frac{\partial^2}{\partial \tilde{\xi}^2} W - 2\tilde{\xi} \frac{\partial}{\partial \tilde{\xi}} W + 2\tilde{\nu} W = 0, \quad \tilde{\nu} = -\left(\frac{\beta}{G} + 1\right). \tag{12.75}$$

In contrast to the standard Hermite differential equation, $\tilde{\nu}$ does not necessarily have to be a natural number. If we go a little beyond the discussion in [212] and perform a further final substitution of the variables according to $z := \tilde{\xi}^2$ with $F(z) = F(\tilde{\xi}^2)$, then we can easily show that the differential equation in (12.75) transforms into Kummer's differential equation with the special choice of $b = \frac{1}{2}$ and $a = -\frac{\tilde{\nu}}{2} = \frac{\beta}{G} + 1$:

$$z \frac{\mathrm{d}^2 F}{\mathrm{d}z^2} + \left(\frac{1}{2} - z\right) \frac{\mathrm{d}F}{\mathrm{d}z} + \frac{\tilde{\nu}}{2} F = 0. \tag{12.76}$$

The two linearly independent solutions are given by ${}_1\mathrm{F}_1\left(-\frac{\tilde{\nu}}{2}, \frac{1}{2}, z\right)$ and $U\left(-\frac{\tilde{\nu}}{2}, \frac{1}{2}, z\right)$. This allows to express the self-similar solution of the heat equation $u(x,t)$ in terms of Kummer functions of the first and second kind as

$$u(x,t) = A(t;\tilde{\nu};G)\, \mathrm{e}^{-\frac{\xi^2 G}{2}} \left(c_1(\tilde{\nu}) U\left(-\frac{\tilde{\nu}}{2}, \frac{1}{2}, \frac{\xi^2 G}{2}\right) + c_2(\tilde{\nu})\,{}_1\mathrm{F}_1\left(-\frac{\tilde{\nu}}{2}, \frac{1}{2}, \frac{\xi^2 G}{2}\right)\right), \quad (12.77)$$

with

$$\tilde{\nu} := -\left(\frac{\beta}{G} + 1\right), \quad A(t;\tilde{\nu};G) := A_0 \left(\frac{2G}{L_0^2}(t - t_0)\right)^{-\frac{1}{2}\left(\frac{\tilde{\nu}}{2}+1\right)} \quad \text{and} \quad \xi = \frac{x}{\sqrt{2k_{\mathrm{d}}(t - t_0)}}. \quad (12.78)$$

In [212], they do not perform the last transformation into the Kummer differential equation and this is probably the reason why they do not relate the first independent solution to the Kummer function of the first kind, which automatically occurs in our discussion here. As discussed in [212], in the special case where $\tilde{\nu}$ is an even integer, the two Kummer functions are multiples of each other and can be identified with the Hermite polynomials — they are no longer independent functions. In this case, next to the solution $U\left(-\frac{\tilde{\nu}}{2}, \frac{1}{2}, \frac{\xi^2}{2}\right)$ we can use $\xi\,{}_1\mathrm{F}_1\left(\frac{1}{2} - \frac{\tilde{\nu}}{2}, \frac{3}{2}, \frac{\xi^2}{2}\right)$ as a second independent solution.

Interestingly, as far as $\mathrm{e}^{-\frac{\xi^2 G}{2}}\,{}_1\mathrm{F}_1\left(-\frac{\tilde{\nu}}{2}, \frac{1}{2}, \frac{\xi^2 G}{2}\right)$ is concerned, this is exactly the expression that we obtain in the computation of the semiclassical expectation values in Section 11.3 and Subsection 12.2.1, respectively. Hence, the result of the Fourier transform involved in these computations corresponds to a self-similar solution of the 1+1-dimensional heat equation. The fractional power r of the momentum operator in these semiclassical expectation values determines the scaling behaviour of the time dependent amplitude of the self-similar solution. As can be easily seen and has been already discussed in [212], for $\tilde{\nu} \neq 0$ we obtain a scaling behaviour of the amplitude that differs from the standard $t^{-\frac{1}{2}}$. Carried over to the expectation values of fractional powers of the momentum operator, the case $\tilde{\nu} = 0$ corresponds to the scenario where the operator becomes the identity operator and the expectation value the squared norm of the coherent states. For complexifier coherent states based on the analytic continuation of the heat kernel, this is the expected scaling behaviour of the norm with respect to the classicality parameter that can be identified with the temporal coordinate of the heat equation in this context.

Chapter 13

Kummer's functions and loop quantum gravity — basics

We want to use this chapter to carry over the procedure of computing semiclassical expectation values via Kummer's confluent hypergeometric functions to loop quantum gravity and thereby also recall the respective quantities and nomenclature.

Starting with U(1), we can reduce the coherent states for $\mathrm{U}(1)^3$, (2.164), to obtain as coherent states for U(1)

$$\psi_g^t = \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\frac{t}{2}n^2+pn}\left(\mathrm{e}^{\mathrm{i}\theta(m)}\mathrm{e}^{-\mathrm{i}\theta}\right)^n. \tag{13.1}$$

We again follow the notation of [134]: m denotes the point in phase space the coherent state is peaked around. The subscript g represents the complexified holonomy $g = \mathrm{e}^{p+\mathrm{i}\theta(m)}$, where p is the canonically conjugate of the holonomy $h(A) = \mathrm{e}^{-\mathrm{i}\theta(A)}$. Lastly, the coherent state is labelled by the superscript t, which corresponds to the classicality parameter t. The condensed, basic steps of how we compute semiclassical expectation values of fractional powers of, e.g., the momentum operator then are

$$\begin{aligned}\langle|\hat{p}|^r\rangle_{\psi_g^t} &= \left\|\psi_g^t\right\|^{-2}\sum_{n=-\infty}^{\infty}|tn|^r\mathrm{e}^{-tn^2+2np}\\ &= \left\|\psi_g^t\right\|^{-2}\frac{2\pi}{T}T^r\sum_{N=-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\mathrm{d}x|x|^r\mathrm{e}^{-x^2+\frac{2p}{T}x-\frac{2\pi\mathrm{i}N}{T}x}\end{aligned}$$

$$= \left\|\psi_g^t\right\|^{-2} \frac{2\pi}{T^{1-r}} \sum_{N=-\infty}^{\infty} \Gamma\left(\tfrac{r+1}{2}\right) {}_1\mathrm{F}_1\left(\frac{r+1}{2}, \frac{1}{2}, \left(\frac{p-\pi\mathrm{i}N}{T}\right)^2\right) \tag{13.2}$$

$$\overset{t\to 0}{\approx} |p|^r \left(1 - \frac{r(1-r)}{4}\frac{t}{p^2} - \frac{r(1-r)(2-r)(3-r)}{32}\frac{t^2}{p^4} + \mathcal{O}\left(t^3\right)\right). \tag{13.3}$$

From the first to the second line, we apply the Poisson resummation formula (10.11) by setting $x := \sqrt{t}\,n =: Tn$. We then obtain the integral of a Gaussian function against the r-th root of the absolute value. Using (11.21) we can solve this integral, resulting in a KCHF in the third line. The last step then is obtaining a power series in the classicality parameter t via the asymptotic expansion for large arguments of the KCHF, (11.18). We thereby also inserted the norm of the coherent states,

$$\left\|\psi_g^t\right\|^2 = 2\pi\sqrt{\frac{\pi}{t}} \sum_{n=-\infty}^{\infty} \mathrm{e}^{\frac{p^2}{t}} \mathrm{e}^{-\frac{-\pi^2 n^2}{t}} \mathrm{e}^{2\pi\mathrm{i}n\frac{p}{t}} =: 2\pi\sqrt{\frac{\pi}{t}}\pi\, \mathrm{e}^{\frac{p^2}{t}} (1 + \mathcal{K}_t), \tag{13.4}$$

with $\mathcal{K}_t \overset{t\to 0}{=} 0 + \mathcal{O}(t^\infty)$ — i.e. $\mathcal{K}_t$ can be neglected when considering the semiclassical limit $t \to 0$. The intermediate step between (13.2) and (13.3) reads in some more detail

$$\begin{aligned}(13.2) = {} & \frac{\mathrm{e}^{-\frac{p^2}{t}}}{2\pi\sqrt{\frac{\pi}{t}}(1+\mathcal{K}_t)} \frac{2\pi}{T^{1-r}} \sum_{N=-\infty}^{\infty} \Gamma\left(\tfrac{1+r}{2}\right)\Gamma\left(\tfrac{1}{2}\right) \cdot \\ & \cdot \left[\frac{\mathrm{e}^{\pm\pi\mathrm{i}\frac{r+1}{2}}}{\Gamma\left(-\frac{r}{2}\right)} \left(\left(\frac{p-\pi\mathrm{i}N}{T}\right)^2\right)^{-\frac{r+1}{2}} \sum_{n=0}^{\infty} \frac{\left(\frac{r+1}{2}\right)_n \left(1+\frac{r}{2}\right)_n}{n!} \left(-\left(\frac{p-\pi\mathrm{i}N}{T}\right)^2\right)^{-n} + \right. \\ & \left. + \frac{1}{\Gamma\left(\frac{r+1}{2}\right)} \mathrm{e}^{\left(\frac{p-\pi\mathrm{i}N}{T}\right)^2} \left(\left(\frac{p-\pi\mathrm{i}N}{T}\right)^2\right)^{\frac{r}{2}} \sum_{n=0}^{\infty} \frac{\left(-\frac{r}{2}\right)_n \left(\frac{1-r}{2}\right)_n}{n!} \left(\left(\frac{p-\pi\mathrm{i}N}{T}\right)^2\right)^{-n}\right].\end{aligned} \tag{13.5}$$

To go from here to (13.3), we first of all notice that the norm of the coherent state adds another Gaussian to the expression: $\exp\left(-p^2/t\right)$. While this Gaussian makes the first series within the square brackets above vanish for $t \to 0$, the second one is already scaled by the inverse of a Gaussian in $\frac{p-\pi\mathrm{i}N}{T}$. The remaining Gaussian $\exp\left(-\pi^2 N^2/t\right)$ implies that only the term with $N = 0$ contributes for $t \to 0$. This does not only simplify the calculations but also eliminates the imaginary part of $\left((p-\pi\mathrm{i}N/T)^2\right)^{r/2}$, which reduces to the prefactor and zeroth order contribution $|p/T|^r$. We thereby arrived at (13.3) and notice that the steps as well as the reduction to only one series and $N = 0$ resembles the quantum mechanical case of Section 11.3, confer (11.30).

The last aspect of this note on the basics of the procedure shall be the transition to $\mathrm{U}(1)^3$. Computing the expectation value of the momentum operator now means considering $\hat{p}_I^i$, for a specific edge e_I of the graph and a specific choice i for the corresponding copy of U(1). With the coherent states for $\mathrm{U}(1)^3$ being just the edge- and U(1)-copy-wise product of the coherent states of U(1), confer (2.164), the expectation value can be deduced from the respective result of U(1) in a rather straightforward manner:

$$\begin{aligned}\langle\left|\hat{p}_{I_0}^{i_0}\right|^r\rangle_{\Psi_m} &= \|\Psi_m\|^{-2} \sum_{\left\{n_I^i\right\}\in\mathbb{Z}} \left|t n_{I_0}^{i_0}\right|^r \mathrm{e}^{\sum_{i,I}\left(-t\left(n_I^i\right)^2+2n_I^i p_I^i\right)} \\ &= \|\Psi_m\|^{-2}\left(\frac{2\pi}{T}\right)^{3M} T^r \sum_{\left\{N_I^i\right\}\in\mathbb{Z}} \int_{-\infty}^{\infty} \mathrm{d}^{3M}x_I^i \, |x_{I_0}^{i_0}|^r \; \mathrm{e}^{\sum_{i,I}\left(-\left(x_I^i\right)^2+\frac{2p_I^i}{T}x-\frac{2\pi\mathrm{i}N_I^i}{T}x_I^i\right)} \\ &\overset{t\to 0}{\approx} \left|p_{I_0}^{i_0}\right|^r\left(1-\frac{r(1-r)}{4}\frac{t}{\left(p_{I_0}^{i_0}\right)^2}-\frac{r(1-r)(2-r)(3-r)}{32}\frac{t^2}{\left(p_{I_0}^{i_0}\right)^4}+\mathcal{O}\left(t^3\right)\right).\end{aligned} \tag{13.6}$$

We noticed in the second line that only the integral over $x_{I_0}^{i_0}$ is not of standard Gaussian type. Hence, $3M-1$ many integrals can be easily solved, obtaining $\sqrt{\pi}\exp\left(-\left(p_I^i-\pi\mathrm{i}N_I^i/T\right)^2\right)$ a time. For the remaining integral, the steps are the same as the ones leading to (13.3) for U(1). Accordingly, the result looks the same and we only need to consider the labelling of the momentum, i.e. i_0 for the chosen copy of U(1) the momentum should be evaluated on as well as the edge e_I.

This should suffice as an overview on the basics for computing semiclassical expectation values in loop quantum gravity with the help of Kummer's confluent hypergeometric functions. This mechanism offers i.a. a concise way of computing expectation values of rational powers of the momentum operator that results in the classical limit for zeroth order in t. Last but not least, we want to note that [135] were in fact also able to reproduce this zeroth order, making use of the Hamburger momentum problem, but had to constrain r to $r=\frac{n}{2}, n\in\mathbb{N}$, and did not further examine the higher order correction terms.

Chapter 14

Kummer's functions and loop quantum gravity — cubic graphs

We introduced in the last chapter a tool for computing semiclassical expectation values in loop quantum gravity that can also be applied to operators like the momentum operator to the power of a rational number. This chapter now covers the application of that procedure to the computation of semiclassical expectation values of the class of operators $\hat{q}^{i_0}_{I_0}(r)$, (10.14), while focusing on the case of cubic graphs. First of all, we will notice that determining the expectation value for cubic graphs corresponds to the computation of the *basic building block* of the general expectation value, so it is the next logical step to do. We will also be able to perform the computations analytically for this simplified scenario — at least for $t \to 0$ without also considering $p \to 0$. When simultaneously addressing the limit $p \to 0$, it will turn out that we are indeed forced to use estimates.

14.1 The setup

During our treatment of cubic graphs, we will have in mind the work of [64] where also semiclassical expectation values of the class of operators $\hat{q}^{i_0}_{I_0}(r)$ were considered for cubic graphs. However, they did use a slightly different notation and we will also highlight these difference in the course of this section about the setup.

For cubic graphs, the volume operator evaluated on a vertex v reads

$$\hat{V}_{\gamma,v} = {\ell_{\mathrm{P}}}^3 \sqrt{\left| \epsilon_{jkl} \frac{\hat{X}^j_{v,e_1^+} - \hat{X}^j_{v,e_1^-}}{2} \cdot \frac{\hat{X}^k_{v,e_2^+} - \hat{X}^k_{v,e_2^-}}{2} \cdot \frac{\hat{X}^l_{v,e_3^+} - \hat{X}^l_{v,e_3^-}}{2} \right|}, \tag{14.1}$$

where we mainly adopted the notation of [64] and only replaced their notation $\widehat{Y}^e_j$ for the right-invariant vector fields of U(1) with our already previously used $\hat{X}^j_{v,e}$. We note that the three factors $\frac{1}{2}$ combine to one part of the numerical prefactor $\frac{1}{48}$ that is included in the volume operator according to (2.106). Considering also a factor of $\frac{1}{6}$, which comes from fixing the order of the edges for cubic graphs, we ultimately obtain the full $\frac{1}{48}$.

Most notably, (14.1) does not include a sum over edges anymore. Due to the regular structure of cubic graphs, we can explicitly write down the combination of all edges that we combined to three pairs of one ingoing and one outgoing edge each: $e^{\pm}_{I=1,2,3}$. This results directly in the eigenvalue

$$\lambda^r\left(\{x^j_J\}\right) = t^{\frac{3r}{2}} \sqrt{\left| \epsilon_{jkl} \frac{x^j_{+,1} - x^j_{-,1}}{2} \cdot \frac{x^k_{+,2} - x^k_{-,2}}{2} \cdot \frac{x^l_{+,3} - x^l_{-,3}}{2} \right|}^{\,r}, \tag{14.2}$$

of $\frac{1}{a^{3r}}\hat{V}^r$, where we factored out the arbitrary length scale a to only work with the classicality parameter t[64, cf. eq. (4.6) therein]. Up to now, in the semiclassical expectation value including the eigenvalues above, we have all 18 charges — 6 edges and 3 copies of U(1) — in both Gaussian functions as well as the absolute value within λ^r. We can reduce the number of charges within λ^r by a factor of one half by substituting

$$x^-_{Jj} := \frac{x^j_{+,J} - x^j_{-,J}}{2} \quad \text{and} \tag{14.3}$$

$$x^+_{Jj} := \frac{x^j_{+,J} + x^j_{-,J}}{2}. \tag{14.4}$$

For the Gaussian functions stemming from the coherent states, this means that those six of them that contain the x^+_{Jj} can be easily integrated as they are of normal Gaussian form. The remaining nine integrals over x^-_{Jj} then contain

$$\lambda^r\left(\{x^-_{Jj}\}\right) = t^{\frac{3r}{2}} \sqrt{\det(x^-_{Jj})}^{\,r} \tag{14.5}$$

additionally to the Gaussian functions. With all this as well as the norm of the coherent states, we can state the form of the expectation values of interest by comparing (10.14) with equation (4.20) of [64]:

$$\frac{2^N}{t^N}\langle\prod_{k=1}^{N}\hat{q}^{j_k}_{J_k}(r)\rangle_{\Psi_m} = (1\pm\mathcal{K}_t)\sqrt{\frac{2}{\pi}}^9\int\limits_{-\infty}^{\infty} \mathrm{d}^9x\ \mathrm{e}^{-2\sum_{Jj}\left(x^j_J\right)^2}\prod_{k=1}^{N}\lambda^r_{J_kj_k}\left(\left\{x^j_J+\tfrac{p^j_J}{T}\right\}\right), \tag{14.6}$$

with the eigenvalues $\lambda^r_{J_kj_k}$ reading

$$\lambda^r_{J_kj_k}\left(\left\{x^j_J+\tfrac{p^j_J}{T}\right\}\right) := 2\frac{\lambda^r\left(\left\{x^j_J+\frac{p^j_J}{T}\right\}\right)-\lambda^r\left(\left\{x^j_J+\frac{p^j_J}{T}+\frac{T}{2}\delta^{jj_k}_{JJ_k}\right\}\right)}{t}. \tag{14.7}$$

Note that we will not use the superscript label $^-$ within x^-_{Jj} and p^-_{Jj} anymore in order to have a more concise notation. We furthermore used the previously introduced $(1\pm\mathcal{K}_t)$ instead of the prefactor of [64]. Another difference in notation compared to [64] is that we do not include the label σ in λ^r that specifies the orientation of an edge. For cubic graphs, as [64] states as well, the orientation has no influence anymore. Last, the prefactor $\frac{2}{t}$ stems from an additional factor of 2 due to the regularisation of the Poisson bracket [234] and the substitution of τ_i by i during the replacement of SU(2) by $U(1)^3$ and the quantisation that implies a division by $\hbar$. In [64], this prefactor is part of an alternative definition of the class of operators $\hat{q}^{i_0}_{I_0}(r)$, as can be seen in equation (4.2) of that reference.[1]

If we now set $N=1$ in (14.6), we call the resulting expression the *basic building block* of the kind of semiclassical expectation values (10.14) as it describes the most simple configuration: The difference of two determinants of two charge matrices, where the charge matrix of the subtrahend experiences a shift $+\frac{T}{2}\delta^{ii_k}_{JJ_k}$ in its element (j_k, J_K). This is the setup for the next section where we will perform the analytical computation of this semiclassical expectation value.

14.2 Analytical computation of $\langle q \rangle$

We now want to perform the computation of the previously introduced semiclassical expectation values. For not overcomplicating the notation, we get rid of one pair of

[1] We note that the 2 is supposed to be in the nominator there and when it comes to the regularisation of the Poisson bracket, the additional factor of 2 was not used.

variables: (i_0, I_0), which specify the holonomy included in $\hat{q}^{i_0}_{I_0}(r)$. Instead, we fix this holonomy to be in $i_0 = 1$ and $I_0 = 1$. This is not a special case at all as we will soon see. The starting point for computing the semiclassical expectation value of $\hat{q}^1_1(r)$ then reads

$$\frac{2}{t}\langle\hat{q}^1_1(r)\rangle_{\Psi_m} =$$
$$= \frac{2}{t}\frac{{\ell_\mathrm{P}}^{6r}}{a^{6r}\|\Psi_m\|^2}\sum_{\{N^i_I\}\in\mathbb{Z}}\left(\tfrac{2\pi\sqrt{2}}{T}\right)^9\int\limits_{-\infty}^{\infty}\mathrm{d}^9x^i_I\ \mathrm{e}^{2\sum_{Ii}\left(-\left(x^i_I\right)^2+2\frac{p^i_I-\pi\mathrm{i}N^i_I}{T}x^i_I\right)}\frac{\left(|\det X|^r-|\det\widetilde{X}|^r\right)}{T^{3r}}$$
$$= \frac{2}{t}\frac{\left(\frac{2\pi\sqrt{2}}{T}\right)^9T^{3r}}{\|\Psi_m\|^2}\sum_{\{N_i\}\in\mathbb{Z}}\mathrm{e}^{\sum_i 2\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\int\limits_{-\infty}^{\infty}\mathrm{d}^9x_i\ \mathrm{e}^{-2\sum_i\left(x_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\left(|\det X|^r-|\det\widetilde{X}|^r\right), \tag{14.8}$$

where

$$X := \begin{pmatrix} x^1_1 & x^2_1 & x^3_1 \\ x^1_2 & x^2_2 & x^3_2 \\ x^1_3 & x^2_3 & x^3_3 \end{pmatrix} =: \begin{pmatrix} x_1 & x_2 & x_3 \\ x_4 & x_5 & x_6 \\ x_7 & x_8 & x_9 \end{pmatrix} \quad \text{and} \quad \widetilde{X} := \begin{pmatrix} x_1+\frac{T}{2} & x_2 & x_3 \\ x_4 & x_5 & x_6 \\ x_7 & x_8 & x_9 \end{pmatrix}. \tag{14.9}$$

We can now clearly see what happens had we not started with $\hat{q}^1_1(r)$ but any other choice of (i_0, I_0): $\widetilde{X}$ would have the shift not in its $(1,1)$-component but the one corresponding to the choice of (i_0, I_0). However, we can of course rearrange the matrix elements accordingly, ending up again with the shift in the $(1,1)$-component. Alternatively, all the upcoming steps can also be performed for any other matrix element than the $(1,1)$ one. Our final result will also be of a form that it is straightforwardly transferable to the general case.

In (14.8), we used $\int_{-\infty}^{\infty}\mathrm{d}^9x^i_I$ as an abbreviation for $\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\mathrm{d}x^1_1\mathrm{d}x^2_1\cdots\mathrm{d}x^3_3$ and $\sum_{Ii}$ for $\sum_{\substack{i=1,2,3\\ I=1,2,3}}$. Note that from the second line onwards, we do no longer use i as a label for the U(1)-copy, but as an index for the matrix elements x_i, p_i and N_i — which are just the $x_{\bar{J}j}$, $p_{\bar{J}j}$ and $n_{\bar{J}j}$ of [64]. As another point of reducing the complexity of our upcoming expressions, we use plain r as the exponent of $|\det X|^r$. To account for the correct dimensions, we accordingly changed ${\ell_\mathrm{P}}^{3r}$ and a^{3r} to ${\ell_\mathrm{P}}^{6r}$ and a^{6r}, respectively.

In general, our starting point is just right after having performed the Poisson resummation formula. We did this via the introduction of $x_i := Tn_i$, with $T^2 := t$, just as before.

To start with the integration procedure, we first tackle the x_1-integration:

$$\int_{-\infty}^{\infty} \mathrm{d}x_1 \; \mathrm{e}^{-2\left(x_1 - \frac{p_1 - \pi \mathrm{i} N_1}{T}\right)^2} |\det X|^r = \\ = \int_{-\infty}^{\infty} \mathrm{d}x_1 \; \mathrm{e}^{-2\left(x_1 - \frac{p_1 - \pi \mathrm{i} N_1}{T}\right)^2} |x_1 x_5 x_9 + x_2 x_6 x_7 + x_3 x_4 x_8 - x_1 x_6 x_8 - x_2 x_4 x_9 - x_3 x_5 x_7|^r. \tag{14.10}$$

We want to have an expression at hand that is of the form (11.20) and notice that we can achieve this via the substitution

$$x_1' \coloneqq \det X, \tag{14.11}$$

$$x_{2,\dots,9}' \coloneqq x_{2,\dots,9}, \tag{14.12}$$

where

$$\det\left(\frac{\mathrm{d}x'}{\mathrm{d}x}\right) = \det \begin{pmatrix} x_5 x_9 - x_6 x_8 & x_6 x_7 - x_4 x_9 & x_4 x_8 - x_5 x_7 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = x_5 x_9 - x_6 x_8. \tag{14.13}$$

With this, we can express the x_1-integration as

$$\int_{-\infty}^{\infty} \mathrm{d}x_1 \; \mathrm{e}^{-2\left(x_1 - \frac{p_1 - \pi \mathrm{i} N_1}{T}\right)^2} |\det X|^r = \\ = \int_{-\infty}^{\infty} \mathrm{d}x_1' \; \mathrm{e}^{-2\left(\frac{x_1'}{x_5' x_9' - x_6' x_8'} + \frac{x_3' x_5' x_7' + x_2' x_4' x_9' - x_2' x_6' x_7' - x_3' x_4' x_8'}{x_5' x_9' - x_6' x_8'} - \frac{p_1 - \pi \mathrm{i} N_1}{T}\right)^2} \frac{|x_1'|^r}{|x_5' x_9' - x_6' x_8'|} \\ =: \int_{-\infty}^{\infty} \mathrm{d}x_1' \; \mathrm{e}^{-2\left(\frac{x_1'}{x_5' x_9' - x_6' x_8'} + x_0\right)^2} \frac{|x_1'|^r}{|x_5' x_9' - x_6' x_8'|}. \tag{14.14}$$

Therein, we obtained the rather long offset x_0 that results from inserting the inversion $x_1 = x_1(x_1', \dots, x_9')$ of (14.11). During our treatment of the remaining integrals, confer Appendix B, we obtain similar expressions that we abbreviate straight away by $a, b, \sigma, \tilde{\sigma}$, etc. Through the substitution, also the term $|x_5'x_9' - x_6'x_8'|$ entered our formulae. With this difference being found in the denominator, we could in principle run into problems when it approaches, or equals, 0. However, we notice that the preceding Gaussian is also in $1/(x_5'x_9'-x_6'x_8')$ and therefore suppresses those points and regions. Even during the upcoming integrations of x_5'-, x_9'-, x_6'- & x_8' we will not have trouble with this expression as the result of the x_1'-integration will neatly merge with it into a once again integrable expression.

We can now combine (11.20) and (11.22) to obtain our basic integration rule

$$\int_{-\infty}^{\infty} \mathrm{d}x \; \mathrm{e}^{-2\left(\frac{x}{s}-x_0\right)^2} |x|^r = (\sqrt{2})^{-1-r} |s|^{1+r} \Gamma\left(\tfrac{1+r}{2}\right) \mathrm{e}^{-2(x_0)^2} {}_1\mathrm{F}_1\left(\frac{1+r}{2}, \frac{1}{2}, 2(x_0)^2\right), \tag{14.15}$$

which applied to the x_1-integration results in

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}x_1 \; \mathrm{e}^{-2\left(x_1 - \frac{p_1 - \pi \mathrm{i} N_1}{T}\right)^2} |\det X|^r &= \int_{-\infty}^{\infty} \mathrm{d}x_1' \; \mathrm{e}^{-2\left(\frac{x_1'}{x_5'x_9'-x_6'x_8'}+x_0\right)^2} \frac{|x_1'|^r}{|x_5'x_9' - x_6'x_8'|} \\ &= \frac{|x_5'x_9' - x_6'x_8'|^{1+r}}{|x_5'x_9' - x_6'x_8'|} (\sqrt{2})^{-1-r} \Gamma\left(\tfrac{1+r}{2}\right) \mathrm{e}^{-2(x_0)^2} {}_1\mathrm{F}_1\left(\frac{1+r}{2}, \frac{1}{2}, 2(x_0)^2\right). \end{aligned} \tag{14.16}$$

As expected, there is no dependency on $x_1{}^{(\prime)}$ left, but instead p_1 entered our formulae. It is contained in the offset x_0, together with all the remaining integration variables $x_2', \ldots, x_9'$. For those, we additionally have the Gaussian functions, which we just ignored during the isolated treatment of the $x_1{}^{(\prime)}$-integration. We now continue in a similar fashion with the integral over x_5', where we combine the result of the first integration, (14.16), with the Gaussian in x_5':

$$\int_{-\infty}^{\infty} \mathrm{d}x_5' \; \mathrm{e}^{-2\left(x_5' - \frac{p_5 - \pi \mathrm{i} N_5}{T}\right)^2} |x_5'x_9' - x_6'x_8'|^r (\sqrt{2})^{-1-r} \Gamma\left(\tfrac{1+r}{2}\right) \mathrm{e}^{-2(x_0)^2} {}_1\mathrm{F}_1\left(\frac{1+r}{2}, \frac{1}{2}, 2(x_0)^2\right).$$

When it comes to the first two factors of the integrand, it looks as if we could apply the same integration rule as before. However, via x_0 enter two additional factors that contain x_5' and with one being the KCHF resulting from the x_1'-integration, this thwarts any analytical integration. We are therefore forced to proceed differently and first examine x_0,

$$x_0 = f\left(\left\{x_{i\setminus 1}'\right\}\right) - \frac{p_1 - \pi \mathrm{i} N_1}{T}, \tag{14.17}$$

realising that it can be understood as being built up by two different parts: While $f\big(\{x'_{i\setminus 1}\}\big)$ collects all dependencies on the remaining integration variables, the second part is the offset $\frac{p_1-\pi\mathrm{i}N_1}{T}$ of the initial Gaussian in x_1. Having in mind that we are ultimately interested in the semiclassical limit of the expectation value, i.e. consider small t and small T accordingly, we can apply the asymptotic expansion for large arguments of the KCHF, (11.18), as at least the part $\frac{p_1-\pi\mathrm{i}N_1}{T}$ of the argument of the KCHF will indeed be large. Doing so results in

$$\begin{aligned}
&\int\limits_{-\infty}^{\infty} \mathrm{d}x_1\ \mathrm{e}^{-2\left(x_1-\frac{p_1-\pi\mathrm{i}N_1}{T}\right)^2}\left|\det X\right|^r = \\
&\quad = \left|x'_5x'_9 - x'_6x'_8\right|^r (\sqrt{2})^{-1-r}\Gamma\big(\tfrac{1+r}{2}\big)\mathrm{e}^{-2(x_0)^2}{}_1\mathrm{F}_1\left(\frac{1+r}{2},\frac{1}{2},2(x_0)^2\right) \\
&\quad \overset{t\to 0}{\approx} \frac{1}{\sqrt{2}}\left|x'_5x'_9 - x'_6x'_8\right|^r\Gamma\big(\tfrac{1}{2}\big)\big((x_0)^2\big)^{\frac{r}{2}}\left(1-\frac{r(1-r)}{4}\frac{(x_0)^{-2}}{2}+\mathcal{O}\big((x_0)^{-4}\big)\right), \quad (14.18)
\end{aligned}$$

where as before only one series of the expansion hat to be considered due to a damping Gaussian prefactor — here in x_0. We see that we obtain a power series in integer powers but also keep track of the initial exponent r. In the literature [64–66], Taylor expansions or the application of estimates leads to results that are also, but there indeed exclusively power series with integer powers and the non-integer exponent of the initial operator is lost, i.e. the exponent r of V^r within $\hat{q}^{i_0}_{I_0}(r)$. So if we manage to preserve this rational exponent in the integration variables, we will likely end up with a final result that also features the initial exponent in the p_i. However, the expression above is still not integrable in this form as the expressions including x_0 are too involved. Taking a look at (14.8), we see that we still have an additional Gaussian in $\frac{p_1-\pi\mathrm{i}N_1}{T}$ that originates from completing the square in x_1 of the initial Gaussian function. This Gaussian will also cause a damping in the semiclassical limit, but via dividing by the norm of the state, we will ultimately eliminate the part in p_1 — and all other p_i —, confer (B.51). Hence, the Gaussian in N_1 is left and as we already performed the integration over $x_1{}^{(\prime)}$, another factor that eliminates this function cannot come up. This leads us to the conclusion that only the contribution $N_1 = 0$ will not be suppressed when taking the limit of $t \to 0$. This reduction to $N_i = 0$, as already mentioned earlier, is a recurring feature also in the literature (cf. [64, 66, 134, 135]) and the very reason for applying the Poisson resummation formula.

With $N_1 = 0$, we have $x_0\big|_{N_1=0} \in \mathbb{R}$ and therefore

$$\left((x_0)^2\right)^{\frac{r}{2}}\bigg|_{N_1=0} = |x_0|^r. \tag{14.19}$$

As we also face another absolute value to the power of r, we may combine those:

$$\begin{aligned} |x'_5x'_9 - x'_6x'_8|^r|x_0|^r &= \left|x'_3x'_5x'_7 + x'_2x'_4x'_9 - x'_2x'_6x'_7 - x'_3x'_4x'_8 - (x'_5x'_9 - x'_6x'_8)\frac{p_1}{T}\right|^r \\ &=: \left|x'_5\Big(x'_3x'_7 - x'_9\frac{p_1}{T}\Big) + \tilde{x}_0\right|^r. \end{aligned} \tag{14.20}$$

From the first line we infer that we actually face a similar situation as right at the beginning — the only difference being the replacement of x_1 by $\frac{p_1}{T}$, while the structure itself is very much like a determinant. However, additionally to this familiar expressions, we also face a power series that contains another term $\sim (x_0)^{-2}$. Concerning this term, we realise that it is a power series in x_0 where we are actually interested in a power series directly in t or T, respectively:

$$1 - \frac{r(1-r)}{4}\frac{(x_0)^{-2}}{2} \approx 1 - \frac{r(1-r)}{4}\frac{T^2}{2{p_1}^2} + \mathcal{O}\big(T^3\big) =: \mathcal{S}. \tag{14.21}$$

Proceeding to a power series in T therefore results in x_i-independent correction terms up to T^2 and we can therefore continue with the remaining integrations: The integral over x'_5 can now be solved by the same steps as the ones we performed for the integral over x'_1. We want to point out that in the Taylor expansion (14.21), the higher order terms $\mathcal{O}(T^3)$ do indeed contain the remaining integration variables. So if we are interested in higher order correction terms, we will have to deal with those in a different way than the previously applied one (the first choice would be to try a new kind of substitution). For the scope of this work, we will only concentrate on the first correction terms and therefore leave this question open.

Continuing with the integral over x'_5, we take along some of the arisen prefactors and face solving

$$\Gamma\big(\tfrac{1}{2}\big)\mathcal{S}\int\limits_{-\infty}^{\infty} \mathrm{d}x'_5\ \mathrm{e}^{-2\left(x'_5 - \frac{p_5 - \pi \mathrm{i} N_5}{T}\right)^2}\left|x'_5\Big(x'_3x'_7 - x'_9\frac{p_1}{T}\Big) + \tilde{x}_0\right|^r.$$

With this integral resembling the one for x'_1, (14.10), we start in a similar way by substituting

$$x''_5 := x'_5\Big(x'_3 x'_7 - x'_9 \frac{p_1}{T}\Big) + \tilde{x}_0, \tag{14.22}$$

$$x''_{2,3,4,6,7,8,9} := x'_{2,3,4,6,7,8,9}, \tag{14.23}$$

$$\det\left(\frac{\mathrm{d}x''}{\mathrm{d}x'}\right) = x'_3 x'_7 - x'_9 \frac{p_1}{T}. \tag{14.24}$$

We thereby end up with integrating the Gaussian function against

$$\frac{|x''_5|^r}{|x'_3 x'_7 - x'_9 \frac{p_1}{T}|}$$

and realise that this is also equivalent to the corresponding expression during the x'_1-integration. With this we refer to Appendix B for the treatment of the remaining integrals. Even though some integrals, or rather results of them, have to be dealt with slightly different, the main procedure will remain the same.

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※ We recap the procedure: First of all, the determinant-like expression within the integrand was substituted as the new integration variable. This gave rise to a new, oblong offset in the corresponding Gaussian function. Yet, this integral was feasible via (11.20) & (11.22) and we end up with a KCHF. Proceeding straight-away with one of the remaining integrals, in turn, was then indeed not possible as the integrand at this point was too intricate due to the KCHF containing all left over integration variables in its argument (amongst other obstacles). However, the argument of the KCHF was also $\sim {}^{p_1}/_{T}$ and as we are interested in the semiclassical limit $T \to 0$, we can therefore make use of the asymptotic expansion for large arguments of the KCHF, (11.18). This resulted in a power series in the inverse of the argument of the KCHF and, consequently, we converted it into a power series in T itself, whose two lowest order contributions were then independent of the remaining integration variables. The last hurdle that had to be overcome was a new factor that entered our formulae in the course of the asymptotic expansion: The argument of the KCHF to the power of ${}^{r}/_{2}$. One issue is that it is a complex number but, as we started with a semiclassical expectation value, the overall expression should still be real. This can be solved by observing the Gaussian prefactors. Realising there is a Gaussian in $(p_1-\pi \mathrm{i} N_1)/T$, we argued that all contributions $N_1 \neq 0$ are suppressed for $T \to 0$ and only the solution $N_1 = 0$ makes up the final result. This also causes the imaginary part of the argument of the KCHF to vanish, turning it into an absolute value to the power of r. With a follow-up combination of this factor with one that came up during the substitution, we end up with an expression quite similar to our starting point, where only x_1 is replaced by p_1/T.

Having illustrated the procedure for the first term of the commutator $\hat{q}^{i_0}_{I_0}(r)$, we now consider the shifted contribution, i.e. the part of (14.8) that contains $|\det \widetilde{X}|^r$. We defined $\widetilde{X}$ in (14.9) as the matrix of all the integration variables but with x_1 being replaced by $x_1 + \frac{T}{2}$. We can then rewrite that part as

$$\int_{-\infty}^{\infty} \mathrm{d}x_1 |\det \widetilde{X}|^r \, \mathrm{e}^{-2\left(x_1 - \frac{p_1 - \pi \mathrm{i} N_1}{T}\right)^2} = \int_{-\infty}^{\infty} \mathrm{d}\tilde{x}_1 |\det X|^r \, \mathrm{e}^{-2\left(\tilde{x}_1 - \frac{p_1 + \frac{T^2}{2} - \pi \mathrm{i} N_1}{T}\right)^2} \tag{14.25}$$

by substituting $\tilde{x}_1 := x_1 + \frac{T}{2}$. Hence, for the shifted contribution, not much changes except for $p_1 \mapsto p_1 + \frac{T}{2}^2$. Accordingly, we can perform the same integration procedure. For the subsequent treatment of the KCHF, i.e. applying the asymptotic expansion for large arguments, we have to be careful due to the additional part being dependent on T. However, we quickly realise that there is no issue with the new term as the important part was that the argument becomes large for $t \to 0$ — and this still holds for $\frac{p_1}{T} + \frac{T}{2}$. In fact, $\frac{T}{2}$ will not even contribute in this limit, at least for this part of the expression. It does nevertheless still change the overall result compared to that of the unshifted expression. Within the absolute value of the offset — (14.19) for the unshifted part — the shift will still be present and the difference of the shifted and unshifted part will therefore not cancel each other.[2] With all remaining integrations being shown in Appendix B, we now only state the final result here. For a graph of cubic topology, the semiclassical expectation value of the operator $\frac{2}{t}\hat{q}^1_1(r)$ reads

$$\frac{2\langle \hat{q}^1_1(r) \rangle_{\Psi_m}}{t} \approx -r \frac{|\det p|^r \Delta^1_1(p)}{\det p} + \mathcal{F}(\{p_i\})\, t + \mathcal{O}\left(t^{\frac{3}{2}}\right). \tag{14.26}$$

[2] All details behind this are explained in more detail in Appendix B.

All the new variables therein emerge peu à peu during the integration procedure covered in Appendix B. First of all, $\det p$ denotes the determinant of the matrix of all momenta p_I^i. We already saw during the x_1-integration that the obtained result corresponds to replacing $x_1 \mapsto p_1$ in the initial expression, so it is of no surprise that the final result accordingly contains $\det X|_{x_I^i \mapsto p_I^i}$. Furthermore, we have $\Delta_1^1(p) := p_2^2 p_3^3 - p_3^2 p_2^3 \equiv p_5 p_9 - p_6 p_8$ — the minor of the matrix of all momenta with respect to $p_1^1 \equiv p_1$. Note that this index is precisely the one of the holonomy that acts within $\frac{2}{t}\hat{q}_1^1(r)$. The last expression, $\mathcal{F}(\{p_i\})$, collects all first order contributions in t. It is a rather evolved function, defined in (B.56) of Appendix B. We note that this order actually contributes with T^4 before dividing the whole expression by t. This may sound suspicious, considering that we only included terms up to $\sim T^2$ in $\mathcal{S}$. However, the final result (B.53) is of such a multiplicative structure that causes all of the terms $\sim T^3$ of $\mathcal{S}$ to ultimately contribute with at least $\mathcal{O}(T^5)$ and we were able to collect all terms up to T^4.

When it comes to the structure of the lowest order contribution within (14.26), we find that it corresponds to the expected result, having mind the expression of the respective classical Poisson bracket. Differentiating a determinant to the power of r with respect to one of its elements, we will obtain that determinant to the power of $r-1$ along the term resulting from the chain rule — which is just the minor of the initial matrix with respect to that element the differentiation considers.

As promised at the beginning of the integration procedure, we can straightforwardly deduce the general result from (14.26) for the holonomy acting on an arbitrary edge I_0 and U(1)-copy i_0:

$$\frac{2\langle \hat{q}_{I_0}^{i_0}(r)\rangle_{\Psi_m}}{t} \approx -r\frac{|\det p|^r \Delta_{I_0}^{i_0}(p)}{\det p} + \widetilde{\mathcal{F}}(\{p_i\})\,t + \mathcal{O}\Big(t^{\frac{3}{2}}\Big). \tag{14.27}$$

We already argued that the initial fixing of $I_0 = 1, i_0 = 1$ was of no mathematical importance whatsoever and indeed, for any other choice of (I_0, i_0) the calculatory steps are just the same, leading to an equivalent result. Of course, $\det p$ will build up as well and only the element of the matrix with respect to which the minor of the matrix is considered will change. The function $\widetilde{\mathcal{F}}(\{p_i\})$ then is of similar shape $\mathcal{F}(\{p_i\})$ was for the specific choice $I_0 = 1, i_0 = 1$ and only the order of how the individual p_i enter the formula, (B.56), changes.

Up to now, we did not need to use any estimates. For cubic graphs, this was also achieved in [64] but via intermediate Taylor expansions that replaced fractional powers by integer ones. In contrast, during the procedure presented here, the powers of the integration variables remain the same up to the considered order in T and the performed Taylor expansions did not change these — compare (14.21) and the remarks following (B.33) and (B.40) within Appendix B. Taking a look at the final result of [64], Theorem 4.2 therein, we consider $N = 1$ and compare this with (14.27) above. The notable difference between the two stems from the fact that [64] already included the influence of the lattice parameter on the fluxes, i.e. lattice fluctuations, while (14.27) contains the fluxes themselves. More details on this will be covered during both Subsection 14.4 and Section 15. The next section focuses on the cosmological singularity, where we can continue with expressions including the fluxes [65, 66].

14.3 The cosmological singularity

Being interested in investigating the cosmological singularity means to consider the limit $p_i = 0$. However, taking a look at (14.26) or (14.27) we notice that this limit is not applicable for those results. This is not surprising, did we perform calculatory steps at earlier stages that were already not applicable for $p_i = 0$: The asymptotic expansion for large arguments of the KCHF, as the name says, requires the KCHF's argument to be large. The important part of the KCHF's argument for this point was $\frac{p_i - \pi i N_i}{T}$. With $p_i = 0$ — and the subsequent realisation that only $N_i = 0$ contributes — this does not hold anymore and we need to deviate from our integration procedure right from the start. For the non-Gaussian part of the integrand of (14.8), we therefore perform estimates to cast it into an expression that is integrable against Gaussian functions:

$$\begin{aligned}
|\det X|^r - \left|\det \widetilde{X}\right|^r &= |\det X|^r - \left|\det X + \frac{T}{2}\Delta_1^1(X)\right|^r \\
&\overset{(16.3)}{\leq} \frac{T^r}{2^r}\left|\Delta_1^1(X)\right|^r = \frac{T^r}{2^r}|x_5 x_9 - x_6 x_8|^r \\
&\overset{(16.4)}{\leq} \frac{T^r}{2^r}\left(|x_5 x_9|^r + |x_6 x_8|^r\right) \\
&\overset{(16.5)}{\leq} \frac{T^r}{2^{2r}}\left(\left(|x_5|^2 + |x_9|^2\right)^r + \left(|x_6|^2 + |x_8|^2\right)^r\right) \\
&\overset{(16.4)}{\leq} \frac{T^r}{2^{2r}}\left(|x_5|^{2r} + |x_9|^{2r} + |x_6|^{2r} + |x_8|^{2r}\right).
\end{aligned} \tag{14.28}$$

The estimates we used here will be explained in more detail later, when they are of key importance for our investigation of the general $\mathrm{U}(1)^3$ scenario in Chapter 16. The result we obtained in (14.28) is indeed integrable against Gaussians and we even face four similar integrals of the form

$$\int\limits_{-\infty}^{\infty} \mathrm{d}x\ \mathrm{e}^{-2x^2}|x|^{2r} = \frac{\Gamma\left(r+\frac{1}{2}\right)}{2^{r+\frac{1}{2}}}. \tag{14.29}$$

The five remaining integrals are of pure Gaussian form but can also be derived from (14.29) for $r=0$. As before, we can reduce the N_i to the contributions $N_i = 0$. In this scenario, the N_i appear exclusively as arguments of Gaussian functions and therefore all terms with $N_i \neq 0$ are exponentially damped. The final result for $p_i = 0$ according to the procedure of (14.28) then is

$$\begin{aligned}\frac{2\langle \hat{q}_1^1(r)\rangle_{\Psi_m}}{t} &\overset{p_i=0}{=} \frac{2}{t}\frac{\left(\frac{2\pi\sqrt{2}}{T}\right)^9 T^{3r}}{\|\Psi_m\|^2}\int\limits_{-\infty}^{\infty}\mathrm{d}^9x_i\ \mathrm{e}^{-2\sum_i (x_i)^2}\Big(|\det X|^r - |\det \widetilde{X}|^r\Big)\\ &\leq \frac{2}{t}\frac{\left(\frac{2\pi\sqrt{2}}{T}\right)^9 T^{4r}}{\|\Psi_m\|^2\, 2^{2r}}\int\limits_{-\infty}^{\infty}\mathrm{d}^9x_i\ \mathrm{e}^{-2\sum_i (x_i)^2}\left(|x_5|^{2r}+|x_9|^{2r}+|x_6|^{2r}+|x_8|^{2r}\right)\\ &= \frac{8}{\sqrt{\pi}\,2^{3r}}\Gamma\left(r+\tfrac{1}{2}\right)t^{2r-1},\end{aligned} \tag{14.30}$$

which we can straightforwardly generalise to

$$\frac{2\langle \hat{q}_{I_0}^{i_0}(r)\rangle_{\Psi_m}}{t} \overset{p_i=0}{\leq} \frac{8}{\sqrt{\pi}\,2^{3r}}\Gamma\left(r+\tfrac{1}{2}\right)t^{2r-1}. \tag{14.31}$$

This was of course possible because a change in the choice of (I_0, i_0) only leads to different x_i being present in (14.28). There are still four integration variables left at the end and the result of the subsequent integrations was independent of the indices of the integration variables.

In general, we therefore do not have a zeroth order contribution — only for $r=\frac{1}{2}$, i.e. when the volume operator is contained within $\hat{q}_1^1(r)$. It is, however, of no surprise that there is no fundamental t^0-term as we did not even obtain one in the quantum mechanical analogue of (11.36). We even get a negative exponent in t if $r<\frac{1}{2}$, so i.a. when we consider

$\sqrt{\hat{\mathrm{V}}}$ — a quite important case in loop quantum gravity. As a result, the limit $t \to 0$ is not well-defined for those scenarios. To compare our result with the literature, we find that the final result (4.7) of [65] divided by t features a t^0 contribution for $r = \frac{4}{3}$, corresponding to $\hat{\mathrm{V}}^{\frac{4}{3}}$ considering their usage of r. As they performed a different procedure based on different estimates, this is already a hint that the final result will drastically depend on the estimates one chooses to apply — even concerning the exponents of the basic variables.

14.4 The semiclassical continuum limit

So far, we considered the semiclassical limit of expectation values of $\frac{2}{t}\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m}$. With $t \to 0$, we expected them to equal $\frac{1}{a^{6r}}\{\int_{e_{I_0}} A^{i_0}(x), V^{2r}_{R_x}\}$, with V_{R_x} as the volume of a region R_x around x. To also access the continuum limit, we now additionally take the limit of a vanishing regularisation parameter a. This combination of the two limits, however, will only be possible for the leading zeroth order in t, while the lattice corrections can in fact cause higher order terms in t to grow tremendously when also considering a vanishing regularisation parameter. In [64], a lattice regularisation parameter $\epsilon = {\ell_{\mathrm{P}}}^{\alpha} a^{1-\alpha}$, with $0 < \alpha < \frac{1}{2}$, was introduced that allows to differ on whether higher order terms do in fact still contribute less than the zeroth order even for small but non-zero t. The authors of [64] then chose $\alpha = \frac{1}{6}$ for the operators they considered. We will now show that as far as the leading order is concerned, we do indeed obtain the correct semiclassical limit via the integration procedure of the previous subsections. More details on lattice fluctuations and an adapted power counting will be presented later in Section 15.1, after (15.17).

We will then be able to verify that our final result (14.27), which was obtained within a setup of a discretised cubic graph, still leads to the expected expression when we additionally take the continuum limit. Note that all higher order contributions can be neglected in this limit as they vanish anyhow. To investigate this question, we have to fall back on the (integration) variables that were the difference of the initial ones, as defined in (14.3). The final result that we derive in more detail in Appendix D then reads

$$\lim_{t\to 0}\frac{2\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m}}{t} = -r\frac{|\det p^-|^r \Delta^{i_0}_{I_0}(p^-)}{\det p^-} = 2\mathrm{i} h^{i_0}_{I_0}\Big\{\big(h^{i_0}_{I_0}\big)^{-1}, V^{2r}(R_{\Box_\epsilon})\Big\} \tag{14.32}$$

and

$$\lim_{\epsilon\to 0}\lim_{t\to 0}\frac{2\langle\hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m}}{t} = \lim_{\epsilon\to 0}\Big(2\mathrm{i}h^{i_0}_{I_0}\Big\{\big(h^{i_0}_{I_0}\big)^{-1}, V^{2r}(R_{\square_\epsilon})\Big\}\Big) = \frac{1}{a^{6r}}\left\{\int_{e_{I_0}} A^{i_0}, V^{2r}(R_x)\right\}. \tag{14.33}$$

So indeed, we do end up with the right classical limit at least for cubic graphs when performing the integration procedure with the help of Kummer's confluent hypergeometric functions and their properties such as the asymptotic expansion for large arguments. During the treatment of Appendix D, two aspects are of great importance: the choice $Z := C_{\mathrm{reg}} = \frac{1}{48}$ for the regularisation constant and an additional factor of 2 after using the Thiemann identity and the regularisation of the Poisson bracket. As we already mentioned, the regularisation constant $C_{\mathrm{reg}} = \frac{1}{48}$ was first introduced in [88] and then validated by an independent consistency check in [89, 90]. The extra factor of 2, meanwhile, is examined in more detail in [234]. As a final note, we point out that these considerations are only valid for graphs of cubic topology. More complex setups, with graphs of higher valence, are not covered by what we just discussed as the regularisation constant $Z = C_{\mathrm{reg}}$ to the power of some rational number r' will still be present in the final result. Only for graphs of cubic topology does $\frac{1}{48}$ match precisely the combinatorics of the $\mathrm{U}(1)^3$ configuration of the edges. We will soon see a counter-example in (15.17).

Chapter 15

Graphs with higher valent vertices

We now turn towards graphs of higher valence — i.e. of more complex structure than the cubic topology we considered previously. For those cubic graphs, the integration procedure based on KCHFs was possible as we had to integrate only the so-called basic building block of the eigenvalue of the operator $\hat{q}^{i_0}_{I_0}(r)$, which consisted of one single determinant that we were able to tackle via appropriate substitutions. For the general setup, we have to consider the whole expression (10.14), which is much more evolved as it is the root of the absolute value of a sum of determinants. Singling out the delicate part of the integrand, i.e. neglecting the Gaussian functions for a start, we face

$$\left|\sum_{IJK}\epsilon(IJK)\epsilon_{ijk}x^i_I x^j_J x^k_K\right|^{\frac{r}{2}} - \left|\sum_{IJK}\epsilon(IJK)\epsilon_{ijk}\big(x^i_I + T\delta^{ii_0}_{II_0}\big)\big(x^j_J + T\delta^{ji_0}_{JI_0}\big)\big(x^k_K + T\delta^{ki_0}_{KI_0}\big)\right|^{\frac{r}{2}}.$$

We can now apply Laplace's formula on the individual sums in the following way:

$$\begin{aligned}\left|\sum_{IJK}\epsilon(IJK)\epsilon_{ijk}x^i_I x^j_J x^k_K\right|^{\frac{r}{2}} &= \\ = \left|x^{i_0}_{I_0}\sum_{JK}\Delta^{i_0}_{I_0}(x_{JK}) - x^{i_0+1}_{I_0}\sum_{JK}\Delta^{i_0+1}_{I_0}(x_{JK}) + x^{i_0+2}_{I_0}\sum_{JK}\Delta^{i_0+2}_{I_0}(x_{JK}) + \det X_{\backslash i_0,I_0}\right|^{\frac{r}{2}}\end{aligned} \tag{15.1}$$

and

$$\left|\sum_{IJK} \epsilon(IJK)\epsilon_{ijk}\left(x_I^i + T\delta_{II_0}^{ii_0}\right)\left(x_J^j + T\delta_{JI_0}^{ji_0}\right)\left(x_K^k + T\delta_{KI_0}^{ki_0}\right)\right|^{\frac{r}{2}} =$$

$$= \left|\left(x_{I_0}^{i_0} + T\right)\sum_{JK} \Delta_{I_0}^{i_0}(x_{JK}) - x_{I_0}^{i_0+1}\sum_{JK} \Delta_{I_0}^{i_0+1}(x_{JK}) + x_{I_0}^{i_0+2}\sum_{JK} \Delta_{I_0}^{i_0+2}(x_{JK}) + \right.$$
$$\left. + \det X_{\setminus i_0, I_0}\right|^{\frac{r}{2}}, \tag{15.2}$$

where we first of all need to make some remarks on the notation: First, we abbreviated $\sum_{I,J,K:\, e_I \cap e_J \cap e_K = v}$ as $\sum_{IJK}$, denoting the sum over all edges e_I, e_J, e_K such that $e_I \cap e_J \cap e_K = v$ and where no edges of a chosen combination of three edges are the same — which is *so far* also guaranteed by $\epsilon(IJK)$. In the same spirit, we use $\sum_{JK}$ for the sum over all edges e_J, e_K such that $e_{I_0} \cap e_J \cap e_K = v \wedge J, K \neq I_0 \wedge J \neq K$. The specific way of applying Laplace's formula was on purpose: The respective first sums within the absolute values on the right hand sides of the two equations above are precisely where the shift caused by the (inverse) holonomy within $\hat{q}_{I_0}^{i_0}(r)$ leaves its trace. As it acts on the element corresponding to the combination of the edge I_0 and U(1)-copy i_0, we have a shift $+T$ in the contribution of $x_{I_0}^{i_0}$ within the second term of the eigenvalue of $\hat{q}_{I_0}^{i_0}(r)$. According to Laplace's formula, the (shifted) matrix element $x_{I_0}^{i_0}(+T)$ is multiplied by the minor of the matrix with respect to $x_{I_0}^{i_0}$, which we call $\Delta_{I_0}^{i_0}(x_{JK})$ — and in the present scenario, we additionally have a sum over all occurring minors that we label by the two involved edges e_J and e_K. The next two contributions then correspond to the remaining summands of Laplace's formula, where the shorthand notation $i_0 + 1$ and $i_0 + 2$ of the superscripts is understood to fulfil periodicity in the indices according to $4 \mapsto 1$ and $5 \mapsto 2$. Finally, the last term $\det X_{\setminus i_0, I_0}$ stands for the collection of all determinants that do not contain the matrix element $x_{I_0}^{i_0}$.

Due to this elaborate structure of the integrand, where we have many contributions that do contain the (shifted) $x_{I_0}^{i_0}$ and many that do not, finding a suitable substitution and proceeding in the same way as we did for cubic graphs seems impossible. Even if we did this for the first integration variable, we would still need to compute all further integrals one by one, too. Accordingly, we had to solve $3M$ integrals for M many edges. What is more, the substitution would have to consider the whole sum and hence, inserting the inversion of the substitution will produce increasingly intricate expressions that we then have to further integrate. This will ultimately lead us to drawing on estimates that allow us to simplify the integrand. Before doing so, there is one further setup where we do in fact not need to rely on estimates — not even on our integration procedure via KCHFs —, but where we in turn can not access the limit $p \to 0$ of the cosmological singularity.

15.1 The Sahlmann–Thiemann approach

We already introduced the work of Sahlmann and Thiemann, who in [64] i.a. developed a mechanism to calculate semiclassical expectation values of the class of operators $\hat{q}^{i_0}_{I_0}(r)$ for graphs of cubic topology. The computation of semiclassical expectation values via Kummer's confluent hypergeometric functions introduced in the previous chapters then was also applicable for this case and hence two questions arise: Can we find a link between the two paths, at least when restricted to cubic graphs? Is it — the other way around — also possible to carry over the method specifically designed to investigate cubic graphs to (more) general scenarios?

While we elaborate on the first question in Section 15.2, the following considerations tackle the possibility of applying the Sahlmann–Thiemann approach on more general graphs than cubic ones. However, we illustrate their procedure using the example of cubic graphs and start with

$$\langle \prod_{k=1}^{N} \hat{q}^{j_k}_{J_k}(r) \rangle_{\Psi_m} = \frac{{\ell_{\mathrm{P}}}^{6rN} |Z_\gamma|^{rN}}{a^{6rN} \|\Psi_m\|^2} \sum_{\{N^i_I\} \in \mathbb{Z}} \left(\frac{2\pi}{T}\right)^9 \int\limits_{-\infty}^{\infty} \mathrm{d}^9 x^i_I \frac{1}{T^{3rN}} \, \mathrm{e}^{\sum_{Ii} \left(\frac{p^i_I - \pi \mathrm{i} N^i_I}{T}\right)^2} \mathrm{e}^{-\sum_{Ii} (x^i_I)^2} \cdot \prod_{k=1}^{N} \left(|\det(X+P)|^r - \left|\det\left(\tilde{X}_k + P\right)\right|^r \right), \tag{15.3}$$

where we again used r instead of $\frac{r}{2}$ to spare us unnecessary complexity in the notation at least in this part. For the matrices in (15.3), we introduced the notation $X + P = \left((x+p)^i{}_I\right)$ with matrix elements $(x+p)^i{}_I = x^i_I + \frac{p^i_I - \pi \mathrm{i} N^i_I}{T}$. The matrix including the shift reads accordingly $\tilde{X}_k = X + \left(\delta^{j_k j} \delta_{J_k J} \frac{T}{m_\gamma}\right)$, where $\left(\delta^{j_k j} \delta_{J_k J} \frac{T}{m_\gamma}\right)$ is a matrix of eight zeroes and $\frac{T}{m_\gamma}$ in entry (j_k, J_k). The variable m_γ allows to cover the general case as well as the special case of cubic graphs simultaneously: We see that $m_\gamma = 2$ reproduces the setup for graphs of cubic topology while we have to stay with $m_\gamma = 1$ in the general case where it is not possible to work with the integration variables $x^\pm$. Finally, we introduced

$Z_\gamma = Z_{\text{comb}}(\gamma) \cdot C_{\text{reg}} = Z_{\text{comb}}(\gamma) \cdot \frac{1}{48}$ that takes over the role of Z before. The reason is that the new Z_γ casts the upcoming formulae into forms that are easier to compare with those from the literature as well as the previous ones for graphs of cubic topology in Subsection 14.2. We still use $C_{\text{reg}} = \frac{1}{48}$ and when it comes to the general case of arbitrary graphs, there is nothing further to do. Hence, we can then set $Z_\gamma = Z = C_{\text{reg}}$, which is just equivalent to $Z_{\text{comb}}(\gamma) = 1$ above. When, in turn, it comes to graphs of cubic topology, the combinatorics of the configuration of the edges allow to factor out $48 \coloneqq Z_{\text{comb}}(\gamma)\big|_{\gamma \text{ is cubic}}$, which is why we did not have any Z or combinatorical prefactors back then — and this was vitally important for being able to recover the semiclassical continuum limit in Section 14.4. For the new Z_γ above, this translates to $Z_\gamma\big|_{\gamma \text{ is cubic}} = 1$.

Beginning with adopting equation (4.21) of [64] to our notation, we face

$$|\det(X+P)|^r - \left|\det\left(\tilde{X}_k + P\right)\right|^r = |\det P|^r \left(\left|\det\left(P^{-1}X + 1\right)\right|^r - \left|\det\left(P^{-1}\tilde{X}_k + 1\right)\right|^r\right). \tag{15.4}$$

as the starting point. The inverse P^{-1} of the matrix P of all p_I^i that we introduced above is built up according to

$$\left(P^{-1}\right)^i{}_I = \frac{1}{\det P}\,\Delta_I^i\left(P^{\text{T}}\right), \tag{15.5}$$

where we again use the letter Δ for the minor $\Delta_I^i\left(P^{\text{T}}\right)$ of P^{T} with respect to entry (i, I):

$$\Delta_I^i\left(P^{\text{T}}\right) \coloneqq \left(P^{\text{T}}\right)^{i+1}{}_{I+1} \cdot \left(P^{\text{T}}\right)^{i+2}{}_{I+2} - \left(P^{\text{T}}\right)^{i+2}{}_{I+1} \cdot \left(P^{\text{T}}\right)^{i+1}{}_{I+2}. \tag{15.6}$$

Note that the shorthand notation of the sub- and superscripts again uses periodicity of the indices.

We can already state two observations at this point: First, the fact that we had to include P^{-1} is the very reason why we will not be able to address the cosmological singularity as setting all p_I^i to zero will not be possible. Second, the minor of the matrix of all the p_I^i right at the start is a promising signal that we will indeed end up with an expression that resembles the classical, differentiation-like result.

When it comes to the T-dependency of the derived quantities of P above, we have $\det P \sim T^{-3}$ and $\Delta_I^i\left(P^{\text{T}}\right) \sim T^{-2}$ as a direct consequence of its elements $(P)^i{}_I = \frac{p_I^i - \pi \mathrm{i} N_I^i}{T}$. Via (15.5), we can then verify the expected $\left(P^{-1}\right)^i{}_I \sim T$. Having these dependencies at hand, we can expand the determinants on the right hand side of (15.4) around the point 1. In doing so and following the argument of [64], we directly neglect all contributions $N_I^i \neq 0$ due to the fact that they contribute with $\mathcal{O}(T^\infty)$ as (15.3) also contains Gaussian functions in $\frac{N_I^i}{T}$. Since up to now there were still imaginary parts $\sim \mathrm{i}N_I^i$ present, we also managed to cast all expressions real. We then follow [64] and proceed by applying the decomposition

$$\det(1+A) = 1 + \operatorname{tr} A + \frac{1}{2}\big((\operatorname{tr} A)^2 - \operatorname{tr} A^2\big) + \det A \tag{15.7}$$

to the difference of the two determinants on the right hand side of (15.4),

$$\left(\det\big(P^{-1}X+1\big)^2\right)^{\frac{r}{2}} - \left(\det\Big(P^{-1}\tilde{X}_k+1\Big)^2\right)^{\frac{r}{2}}.$$

Hence, we in fact need the square of (15.7), which we may as well already at this stage truncate to fourth order in T to obtain

$$\begin{aligned}\det(1+A)^2 &= 1 + 2\operatorname{tr} A + 2(\operatorname{tr} A)^2 - \operatorname{tr} A^2 + (\operatorname{tr} A)^3 - \operatorname{tr} A \cdot \operatorname{tr} A^2 + \\ &\quad + \det A + \operatorname{tr} A \cdot \det A + \frac{1}{4}(\operatorname{tr} A)^4 - \frac{1}{2}(\operatorname{tr} A)^2 \cdot \operatorname{tr} A^2 + \mathcal{O}\big(T^5\big) \\ &=: 1 + z_A + \mathcal{O}\big(T^5\big) \qquad (15.8) \\ \Rightarrow \big(\det(1+A)^2\big)^{\frac{r}{2}} &\approx \sum_{k=0}^{5} \binom{\frac{r}{2}}{k} (z_A)^k + \mathcal{O}\big(T^5\big). \qquad (15.9)\end{aligned}$$

Now, A does not only contain terms $\sim T$, coming from the P^{-1}. For $A = P^{-1}\tilde{X}_k$, there are also terms $\sim T^2$ due to the shift within $\tilde{X}_k$. For this reason as well as for z_A being multiplied with itself, (15.9) contains terms of higher order in T than we in fact want to consider. However, to have clearer formulae, we keep it this way and discard these higher order terms later. We can now insert this decomposition into (15.3), with the result reading

$$\begin{aligned}\langle \prod_{k=1}^{N} \hat{q}_{J_k}^{j_k}(r) \rangle_{\Psi_m} &= \frac{T^{6rN} |Z_\gamma|^{rN}}{\|\Psi_m\|^2} \left(\frac{2\pi}{T}\right)^9 \int_{-\infty}^{\infty} \mathrm{d}^9 x_I^i \frac{1}{T^{3rN}}\, \mathrm{e}^{\sum_{Ii}\left(\frac{p_I^i}{T}\right)^2} \mathrm{e}^{-\sum_{Ii}\left(x_I^i\right)^2} |\det P|^{rN} \cdot \\ &\cdot \prod_{k=1}^{N} \Bigg[r\operatorname{tr}\big(P^{-1}X\big) - r\operatorname{tr}\Big(P^{-1}\tilde{X}_k\Big) + \frac{r}{2}\Big(r\big(\operatorname{tr}\big(P^{-1}X\big)\big)^2 - \operatorname{tr}\big(P^{-1}X\big)^2\Big) -\end{aligned}$$

$$- \frac{r}{2}\Big(r\Big(\mathrm{tr}\Big(P^{-1}\tilde{X}_k\Big)\Big)^2 - \mathrm{tr}\Big(P^{-1}\tilde{X}_k\Big)^2\Big) + r(r-1)\,\mathrm{tr}\big(P^{-1}X\big)\,\mathrm{tr}\big(P^{-1}XP^{-1}\big(\delta^{j_k j}\delta_{J_k J}T\big)\big) -$$
$$- \frac{r^2(r-1)}{2}\big(\mathrm{tr}\big(P^{-1}X\big)\big)^2 \cdot \mathrm{tr}\big(P^{-1}\big(\delta^{j_k j}\delta_{J_k J}T\big)\big) + \mathcal{O}\big(T^5\big)\Big]. \tag{15.10}$$

Therein, we already used the fact that X and $\tilde{X}_k$ differ only in one entry — $\tilde{X}_k = X + \Big(\delta^{j_k j}\delta_{J_k J}\frac{T}{m_\gamma}\Big)$ — to have more concise expressions for the last two terms. We can similarly obtain further simplifications via

$$\mathrm{tr}\big(P^{-1}X\big) - \mathrm{tr}\Big(P^{-1}\tilde{X}_k\Big) = -\,\mathrm{tr}\Big(P^{-1}\Big(\delta^{j_k j}\delta_{J_k J}\tfrac{T}{m_\gamma}\Big)\Big) = -\tfrac{T}{m_\gamma}\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j_k}{}_{J_k} \tag{15.11}$$

and

$$\begin{aligned}
\mathrm{tr}\big(P^{-1}X\big)^2 - \mathrm{tr}\Big(P^{-1}\tilde{X}_k\Big)^2 &= \\
&= -2\,\mathrm{tr}\Big(\big(P^{-1}X\big)\Big(P^{-1}\Big(\delta^{j_k j}\delta_{J_k J}\tfrac{T}{m_\gamma}\Big)\Big)\Big) - \mathrm{tr}\Big(P^{-1}\Big(\delta^{j_k j}\delta_{J_k J}\tfrac{T}{m_\gamma}\Big)\Big)^2 \\
&= -2\,\mathrm{tr}\Big(\big(P^{-1}X\big)\Big(P^{-1}\Big(\delta^{j_k j}\delta_{J_k J}\tfrac{T}{m_\gamma}\Big)\Big)\Big) - \frac{T^2}{m_\gamma^2}\Big(\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j_k}{}_{J_k}\Big)^2,
\end{aligned} \tag{15.12}$$

where we also used

$$\mathrm{tr}\Big(P^{-1}\Big(\delta^{j_k j}\delta_{J_k J}\tfrac{T}{m_\gamma}\Big)\Big) = \tfrac{T}{m_\gamma}\big(P^{-1}\big)^a{}_b\,\delta^{b j_k}\delta_{a J_k} = \tfrac{T}{m_\gamma}\big(P^{-1}\big)_{J_k}{}^{j_k} = \tfrac{T}{m_\gamma}\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j_k}{}_{J_k}. \tag{15.13}$$

With also considering the norm of the state, we therefore now have

$$\begin{aligned}
\langle\prod_{k=1}^{N}\hat{q}^{j_k}_{J_k}(r)\rangle_{\Psi_m} = \frac{T^{6rN}|Z_\gamma|^{rN}}{\sqrt{\pi}^9 T^{3rN}}|\det P|^{rN}\int_{-\infty}^{\infty} \mathrm{d}^9x^i_I\;\mathrm{e}^{-\sum_{Ii}\left(x^i_I\right)^2}\,\cdot \\
\cdot\prod_{k=1}^{N}\Bigg[-r\frac{T}{m_\gamma}\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j_k}{}_{J_k} + \frac{r(1-r)}{2}\frac{T^2}{m_\gamma^2}\Big(\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j_k}{}_{J_k}\Big)^2 - \\
- r^2\frac{T}{m_\gamma}\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j_k}{}_{J_k}\,\mathrm{tr}\big(P^{-1}X\big) + r\,\mathrm{tr}\Big(\big(P^{-1}X\big)\Big(P^{-1}\Big(\delta^{j_k j}\delta_{J_k J}\tfrac{T}{m_\gamma}\Big)\Big)\Big) + \\
+ r(r-1)\frac{T}{m_\gamma}\sum_{j,J}\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j_k}{}_J\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j}{}_J\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j}{}_{J_k}\big(X^j_J\big)^2 - \\
- \frac{r^2(r-1)}{2}\frac{T}{m_\gamma}\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j_k}{}_{J_k}\sum_{j,J}\Big(\big(\big(P^{-1}\big)^{\mathrm{T}}\big)^{j}{}_J\Big)^2\big(X^j_J\big)^2 + \mathcal{O}\big(T^5\big)\Bigg].
\end{aligned} \tag{15.14}$$

We notice that the integration of all terms in the second line of the square bracket against the preceding Gaussians will yield zero as they are linear in one of the integration variables x^i_I.[1] The remaining integrals are then either

$$\int_{-\infty}^{\infty} \mathrm{d}x \; \mathrm{e}^{-x^2} x^2 = \frac{\sqrt{\pi}}{2} \tag{15.15}$$

or of pure Gaussian form — yielding $\sqrt{\pi}$. We will therefore get an overall factor of $\sqrt{\pi}^9$ which eliminates the corresponding factor in the denominator, stemming from the norm of the state.

As a last ingredient, we need

$$P^i{}_I = \frac{p^i_I}{T} \Rightarrow \det P = \frac{\det p}{T^3} \Rightarrow \left(\left(P^{-1}\right)^{\mathrm{T}}\right)^{j_k}{}_{J_k} = T\frac{\Delta^{j_k}_{J_k}(p)}{\det p} \tag{15.16}$$

for the respective factors in (15.14). We can now state our final result, where we have to consider the factor $\frac{2^N}{t^N}$ as we now face an N-fold product of the operators $\hat{q}^{j_k}_{J_k}(r)$:

$$\begin{aligned}
&\frac{2^N \langle \prod_{k=1}^N \hat{q}^{j_k}_{J_k}(r)\rangle_{\Psi_m}}{t^N} = \\
&= \frac{2^N}{t^N}|Z_\gamma|^{rN}|\det p|^{rN}\prod_{k=1}^{N}\Bigg[-r\frac{t}{m_\gamma}\frac{\Delta^{j_k}_{J_k}(p)}{\det p} + \frac{r(1-r)}{2}\frac{t^2}{m_\gamma^2}\frac{\left(\Delta^{j_k}_{J_k}(p)\right)^2}{\left(\det p\right)^2} + \\
&+\frac{r(r-1)}{2}\frac{t^2}{m_\gamma}\sum_{j,J}\frac{\Delta^{j_k}_{J}(p)\Delta^{j}_{J}(p)\Delta^{j}_{J_k}(p)}{\left(\det p\right)^3} - \frac{r^2(r-1)}{4}\frac{t^2}{m_\gamma}\frac{\Delta^{j_k}_{J_k}(p)}{\left(\det p\right)^3}\sum_{j,J}\left(\Delta^j_J(p)\right)^2 + \mathcal{O}\left(t^{\frac{5}{2}}\right)\Bigg] \\
&= (-2r)^N|Z_\gamma|^{rN}\frac{1}{m_\gamma^N}\left(\frac{|\det p|^r}{\det p}\right)^N\prod_{k=1}^{N}\left[\Delta^{j_k}_{J_k}(p)\right] + \mathcal{O}\left(t^{\frac{1}{2}}\right).
\end{aligned} \tag{15.17}$$

With $m_\gamma = 2$ and $Z_\gamma = 1$, we retrieve the same lowest order contribution as we did for cubic graphs — confer (14.26) —, just that we now also cover the more general case of an N-fold product. Therefore, as already mentioned in Section 14.4, it is only for cubic graphs that we can reproduce the semiclassical continuum limit, while for arbitrary graphs we will still have Z_γ in our formulae.

If we now compare (15.17) with the respective result of [64, Theorem 4.2 or (4.45)], we see that the two are expressed differently: While [64] explicitly considers the lattice

[1] We also directly neglected linear contributions from the terms of the third and fourth line.

fluctuations, (15.17) above has those still encoded in the fluxes p_I^i. As we already pointed out during the discussion at the end of Appendix B, Sahlmann and Thiemann [64] introduced $s = t^{\frac{1}{2}-\alpha}$, with $0 < \alpha < \frac{1}{2}$, for also considering the lattice fluctuations. Their resulting power series [64, (4.39)] was then truncated to contributions $\sim s^3 T$, with the first order they neglected being $(sT)^2$. This is the reason why [64, (4.45)] does not contain all the terms that are $\sim t^2$ in the square bracket of (15.17) above (i.e. make up the first higher-order correction terms): the t^2-contribution in the first line of (15.17) corresponds to the $(sT)^2$-term of [64] and is therefore neglected in [64, (4.45)]. While these lattice fluctuations will be present regardless of the choice of α, we kept these higher order terms to be able to compare the results à la Sahlmann–Thiemann with the U(1) and quantum mechanical scenario. There, these two different kind of correction terms share the same order in t or $\hbar$, respectively: Taking a look at (11.30), we see that the expectation value of $|\hat{p}|^r$ in standard quantum mechanics already features fluctuations — and this is not due to a rational exponent but already true for $|\hat{p}|^3$ and higher powers. Proceeding to (11.35), we saw that we obtain two terms that contribute with next-to-leading order $\hbar^2$. Of these, the second one can be found to be the derivative of the fluctuation contribution of (11.30). The first one, in turn, corresponds to the second derivative of the initial expression just like the $\hbar$-contribution corresponds to the first derivative. For the U(1)-case, the same behaviour can be observed if we compare the fluctuations of the expectation value of $|\hat{p}|^r$ in U(1), (12.39), with the second t-contribution of the final result for the expectation value of $\hat{q}^r$, (12.41). We find this also in [64, Theorem 4.3 / eq. (4.48)]: If we differentiate the fluctuation correction of the expectation value of the volume operator as stated there, we get terms $\sim q^{\frac{3r}{2}-3}$. This does indeed fit the correction terms $\sim s^2$ of [64, (4.45)] for $N = 1$.

As a last comment on the general procedure of Sahlmann–Thiemann [64], we note that it *can happen* that there are additional terms in the power series [64, (4.39)], contributing with a power in t between the term $(sx)^2$ and the omitted contributions $\mathcal{O}(sT)$ — depending on the choice of α. Terms $\sim sT \sim t^{1-\alpha}$ will, of course, always be of higher order in t than those $\sim (sx)^2 \sim t^{1-2\alpha}$ — as $0 < \alpha < \frac{1}{2}$ —, but for terms $\sim (sx)^n$ this is not as straightforward: Their t-dependence is $t^{\frac{n}{2}-n\alpha}$, meaning that for a fixed value of α, we have to consider all contributions $(sx)^n$ with $n < \frac{1-\alpha}{1/2-\alpha}$. For the case [64] considers, everything is fine: They chose $\alpha \approx \frac{1}{6}$ (confer [64, comment after (3.12)]), demanding to include all terms $(sx)^n$ with $n < 2.5$. However, if α were approaching $\frac{1}{2}$, we would have to consider all $(sx)^n$ with $n \in 2\mathbb{N}$ and only the contributions with odd n can be neglected for their integral against the preceding Gaussian functions vanishes.

Having introduced the procedure of Sahlmann–Thiemann to compute semiclassical expectation values of (products of) $\hat{q}^{i_0}_{I_0}(r)$ for cubic graphs, we try to extend it to more general scenarios in what follows. Note that this implies $m_\gamma = 1$ and we may therefore as well omit it. The delicate part of the integrand of our starting point now is

$$\prod_{k=1}^{N}\left(\left|\sum_i \det(X_i + P_i)\right|^r - \left|\sum_i \det\left(\tilde{X}_{i,k} + P_i\right)\right|^r\right),$$

where the sum over i is shorthand for summing over the contributions of all triples of edges as in (10.6). As before, we now try to perform a Taylor expansion on this expression. For being able to do so, we first factor out $\det P_1$ and apply the decomposition (15.7). This yields

$$\begin{aligned}\left|\sum_i \det(X_i + P_i)\right|^r = |\det P_1|^r \cdot \Bigg|&1 + \operatorname{tr}\left(P_1{}^{-1}X_1\right) + \frac{1}{2}\left(\left(\operatorname{tr}\left(P_1{}^{-1}X_1\right)\right)^2 - \operatorname{tr}\left(P_1{}^{-1}X_1\right)^2\right) + \\ &+ \det\left(P_1{}^{-1}X_1\right) + \sum_{i\neq 1}\frac{\det P_i}{\det P_1}\Bigg(1 + \operatorname{tr}\left(P_i{}^{-1}X_i\right) + \frac{1}{2}\left(\left(\operatorname{tr}\left(P_i{}^{-1}X_i\right)\right)^2 - \operatorname{tr}\left(P_i{}^{-1}X_i\right)^2\right) + \\ &+ \det\left(P_i{}^{-1}X_i\right)\Bigg)\Bigg|^r \qquad (15.18)\end{aligned}$$

for the unshifted part. We see that we can now indeed perform a Taylor expansion on this expression — just around $1 + \sum_{i\neq 1}\frac{\det P_i}{\det P_1}$ this time. We can also infer from the structure of (15.18) that this contribution will then be eliminated by the equivalent part that one gets for the second contribution of the commutator, the one containing the shift. Hence, we only get terms of higher order than T^1. With an increasing amount of terms per order in T as well as their more and more complex compositions, we consider only the lowest order contributions from now on. In its lowest order, only one term will contribute: the one corresponding to $\operatorname{tr} A$ in (15.7), which became $r \operatorname{tr} A$ after the Taylor expansion (15.9) of the root. We now have to collect this contribution of all possible combinations of three edges, which we ultimately find as

$$\begin{aligned}\prod_{k=1}^{N}\left(\left|\sum_i \det(X_i + P_i)\right|^r - \left|\sum_i \det\left(\tilde{X}_{i,k} + P_i\right)\right|^r\right) = |\det P_1|^{rN} \prod_{k=1}^{N}\Bigg[&r \operatorname{tr}\left(P_1{}^{-1}X_1\right) - \\ - r \operatorname{tr}\left(P_1{}^{-1}\tilde{X}_{1,k}\right) + r\sum_{i\neq 1}\frac{\det P_i}{\det P_1}\operatorname{tr}\left(P_i{}^{-1}X_i\right) - r\sum_{i\neq 1}\frac{\det P_i}{\det P_1}&\operatorname{tr}\left(P_i{}^{-1}\tilde{X}_{i,k}\right) + \mathcal{O}\left(T^3\right)\Bigg]\end{aligned}$$

$$= (-r)^N T^{-3rN+2N} \prod_{k=1}^{N} \left(\sum_i \frac{|\det p_i|^r}{\det p_i} \Delta^{j_k}_{J_k}(p_i) \right) + \mathcal{O}\big(T^{-3rN+2N+1}\big). \tag{15.19}$$

If we now want to compare this with the classical Poisson bracket, we have to multiply the result above by $\frac{2^N}{t^N}$ and get

$$\frac{2^N \langle \prod_{k=1}^N \hat{q}^{j_k}_{J_k}(r) \rangle_{\Psi_m}}{t^N} = (-2r)^N |Z_\gamma|^{rN} \prod_{k=1}^{N} \left(\sum_i \frac{|\det p_i|^r}{\det p_i} \Delta^{j_k}_{J_k}(p_i) \right) + \mathcal{O}\Big(t^{\frac{1}{2}}\Big), \tag{15.20}$$

having in mind that we again used r instead of the initial $\frac{r}{2}$. As expected, we can not fully reproduce the classical result of the Poisson bracket with $Z_\gamma = \frac{1}{48}$ still being part of the expression above. Furthermore, we already noted at the beginning that the entering of P^{-1} into our formulae will likely lead to the limit $p \to 0$ not being accessible — and we see that this turned out to be indeed true.

We close this part on non-estimative approaches for determining semiclassical expectation values of the class of operators $\hat{q}^{i_0}_{I_0}(r)$ with a short recap. First, we used Kummer's confluent hypergeometric functions to develop a computation procedure for the basic building block of these expectation values and were able to apply it to graphs of cubic topology. Second, the procedure Sahlmann and Thiemann introduced in [64] was generalised to applying it to graphs of not necessarily cubic topology. All these investigations where possible without having to rely on estimates — at least unless the cosmological limit of $p = 0$ was considered. Just like the work of Brunnemann and Thiemann, [65, 66], we then had to use estimates as well and obtained a diverging expression when considering both $p \to 0$ and $t \to 0$. The next section will cover a short comparison of the KCHF procedure and the one of Sahlmann and Thiemann, before we delve into estimative approaches in the next chapter, which then is in closer relation to the work of Brunnemann and Thiemann [65, 66].

15.2 Comparison of the KCHF procedure and the one of Sahlmann and Thiemann

Seeing that the two paths — the one of Sahlmann–Thiemann [64] and the one via KCHFs — share scenarios they can be applied to and then yield the same result, the question arises whether there may in fact be a link between the two. For this, we start with the U(1)-case and the integral

$$\mathfrak{I} = \|\Psi\|^{-2} T^r \mathrm{e}^{\frac{p^2}{T^2}} \int\limits_{-\infty}^{\infty} \mathrm{d}x \; \mathrm{e}^{-x^2} \left| x + \frac{p}{T} \right|^r, \tag{15.21}$$

reflecting the basic structure of the integrals we investigate. Note that we directly considered only the contribution of $N = 0$ and the norm of the state then is $\|\Psi\|^2 = \sqrt{\pi}\, \mathrm{e}^{\frac{p^2}{T^2}}$.

Adapting the procedure of Sahlmann–Thiemann [64], we perform a power series expansion of the non-Gaussian part of the integrand as follows:

$$\left| x + \frac{p}{T} \right|^r = \left| \frac{p}{T} \right|^r \cdot \left| 1 + p^{-1} T x \right|^r \approx \left| \frac{p}{T} \right|^r \left(1 + r p^{-1} T x + \frac{r(r-1)}{2} \left(p^{-1} T x \right)^2 + \mathcal{O}\left(T^3 \right) \right). \tag{15.22}$$

Having in mind that the integral of the term linear in x against the preceding Gaussian vanishes, we get

$$\mathfrak{I} = |p|^r \left(1 + \frac{1}{\sqrt{\pi}} \frac{r(r-1)}{2} \frac{T^2}{p^2} \int\limits_{-\infty}^{\infty} \mathrm{d}x \; \mathrm{e}^{-x^2} x^2 + \mathcal{O}\left(T^3 \right) \right) \tag{15.23}$$

$$= |p|^r \left(1 + \frac{r(r-1)}{4} \frac{T^2}{p^2} + \mathcal{O}\left(T^3 \right) \right). \tag{15.24}$$

For the KCHF-procedure, we already presented the general steps several times and applied to (15.21), they read

$$\mathfrak{I} = \|\Psi\|^{-2} T^r \mathrm{e}^{\frac{p^2}{T^2}} \int\limits_{-\infty}^{\infty} \mathrm{d}x \; \mathrm{e}^{-\left(x - \frac{p}{T} \right)^2} |x|^r \tag{15.25}$$

$$= \frac{T^r}{\sqrt{\pi}} \Gamma\left(\tfrac{r+1}{2} \right) {}_1\mathrm{F}_1\left(-\frac{r}{2}, \frac{1}{2}, -\left(\frac{p}{T} \right)^2 \right) \tag{15.26}$$

$$= \frac{T^r}{\sqrt{\pi}} \Gamma\big(\tfrac{r+1}{2}\big)\ \mathrm{e}^{-\frac{p^2}{T^2}} {}_1\mathrm{F}_1\left(\frac{r+1}{2}, \frac{1}{2}, \left(\frac{p}{T}\right)^2\right) \tag{15.27}$$

$$\simeq |p|^r \sum_{n=0}^{\infty} \frac{\big(-\frac{r}{2}\big)_n \big(-\frac{r}{2}+\frac{1}{2}\big)_n}{n!} \big(p^{-1}T\big)^{2n} \tag{15.28}$$

$$= |p|^r \left(1 + \frac{r(r-1)}{4} \frac{T^2}{p^2} + \mathcal{O}\big(T^3\big)\right). \tag{15.29}$$

These are the Kummer transformation (11.11), which we used from the second to the third line, and the asymptotic expansion for large arguments of the KCHF (11.18) from the third to the fourth line. For the latter, we noticed that we have to consider only one of the resulting series — *as usual* by now.

So we see that the two paths do indeed yield the same result and we now try to better understand how the two may be linked. For this, we examine the Taylor series (15.22) and, as stated above, neglect all contributions with odd powers in x. We can do so by modifying the Taylor series to sum over $2n$ instead of n. This allows us to associate the respective numerical prefactors of (15.23) and (15.28), where the ones of the Taylor series are just the generalised binomial coefficients $\binom{r}{n}$. We reformulate these in terms of the falling factorial

$$\begin{aligned} (a)_0^- &= 1, \\ (a)_1^- &= a \quad \text{and} \\ (a)_n^- &= a(a-1)(a-2)\cdots(a-n+1) \end{aligned} \tag{15.30}$$

as

$$\binom{r}{n} = \frac{(r)_n^-}{n!} \tag{15.31}$$

and then have to verify

$$\frac{1}{\sqrt{\pi}} \frac{(r)_{2n}^-}{(2n)!} \int_{-\infty}^{\infty} \mathrm{d}x\ \mathrm{e}^{-x^2} x^{2n} = \frac{\big(-\frac{r}{2}\big)_n \big(-\frac{r}{2}+\frac{1}{2}\big)_n}{n!}. \tag{15.32}$$

This identity is straightforwardly validated via

$$\int_{-\infty}^{\infty} \mathrm{d}x\ \mathrm{e}^{-x^2} x^{2n} = \Gamma\big(n+\tfrac{1}{2}\big) = \frac{(2n)!}{n!4^n}\sqrt{\pi} \tag{15.33}$$

and we can therefore rewrite the asymptotic expansion for large arguments of the KCHF using the contributions of the Taylor expansion of Sahlmann–Thiemann:

$$T^r \mathrm{e}^{-\frac{p^2}{T^2}} {}_1\mathrm{F}_1\left(-\frac{r+1}{2}, \frac{1}{2}, \frac{p^2}{T^2}\right) \simeq |p|^r \cdot \sum_{n=0}^{\infty} \frac{1}{\sqrt{\pi}} \frac{(r)_{2n}}{(2n)!} \left(p^{-1}T\right)^{2n} \int_{-\infty}^{\infty} \mathrm{d}x \; \mathrm{e}^{-x^2} x^{2n}. \tag{15.34}$$

So we can say that in this scenario, the two paths are just two sides of the same medal. This immediately does not hold anymore if we were interested in taking the limit $p \to 0$. Then, introducing p^{-1} during the Sahlmann–Thiemann procedure causes trouble, while using KCHFs would still be feasible with the very definition of the KCHFs, (11.2), directly resulting in a power series in t. For the $\mathrm{U}(1)^3$-scenario, we can not maintain this link between the two procedures. The Sahlmann–Thiemann way still tackles the integrals that one faces after the power series expansion all at once, but the KCHF procedure forced us to perform them iteratively, confer Appendix B.

Chapter 16

Kummer's functions and loop quantum gravity — estimative approaches

In the previous chapter, we were able to determine semiclassical expectation values of the class of operators $\hat{q}^{i_0}_{I_0}(r)$ without the help of estimates. However, if we wanted to consider the limit of the cosmological singularity, i.e. $p \to 0$, we in fact had to rely on estimates. A different procedure by Sahlmann–Thiemann [64] allows to compute similar expectation values for cubic graphs and we saw that also this one can not handle the cosmological singularity as its mechanism relies on the introduction of P^{-1}. As a consequence, we infer that we need to use estimates once we are interested in investigating the initial singularity. As we will see, the choice of which estimates to use is by far not a simple one and it heavily affects the outcome.

We start this part with revisiting an estimative approach introduced by Brunnemann and Thiemann in a pair of two papers [65, 66], which we will directly slightly modify by using KCHFs. While we start with the simple case of one $\hat{q}^{i_0}_{I_0}(r)$, we will then also consider the N-fold product $\langle \prod_{k=1}^{N} \hat{q}^{j_k}_{J_k}(r) \rangle_{\Psi_m}$. The remainder of this chapter then focuses on developing a notion of how to find suitable estimates that allow to improve the obtained result such that the power of both the classicality parameter and the fluxes is conserved.

16.1 Revisiting the approach of Brunnemann and Thiemann

16.1.1 Estimative computation of $\langle \hat{q}^{i_0}_{I_0}(r) \rangle$

Brunnemann–Thiemann established in [65, 66] i.a. a procedure of how to utilise estimates to cast the intertwined integrals one faces when computing semiclassical expectation values of $\hat{q}^{i_0}_{I_0}(r)$ (and products thereof) into ones that then can be solved. We now introduce their procedure using the example of (10.9), which reads

$$\langle \hat{q}^{i_0}_{I_0}(r) \rangle_{\Psi_m} = \frac{1}{\|\Psi_m\|^2 a^{3r}} \sum_{\{n^i_I\} \in \mathbb{Z}} \mathrm{e}^{\sum_{i,I}\left(-t\left(n^i_I\right)^2 + 2p^i_I n^i_I\right)} \ell_{\mathrm{P}}{}^{3r} |Z|^{\frac{r}{2}} \left(\left| \sum_{IJK} \epsilon(IJK) \epsilon_{ijk} n^i_I n^j_J n^k_K \right|^{\frac{r}{2}} - \right.$$
$$\left. - \left| \sum_{IJK} \epsilon(IJK) \epsilon_{ijk} \left(n^i_I + \delta^{ii_0}\delta_{II_0}\right)\left(n^j_J + \delta^{ji_0}\delta_{JI_0}\right)\left(n^k_K + \delta^{ki_0}\delta_{KI_0}\right) \right|^{\frac{r}{2}} \right). \tag{16.1}$$

First, note that we went back to naming the regularisation constant Z. We do not consider special graphs anymore, like cubic ones, so we can as well use $Z_{\mathrm{comb}}(\gamma) = 1 \Rightarrow Z_\gamma = C_{\mathrm{reg}} = \frac{1}{48} =: Z$. An important aspect of our starting point above is that it is before the Poisson resummation, meaning that we still work with the actual $\mathrm{U}(1)^3$-charges n^i_I. For the work of Brunnemann–Thiemann, this was important with their crucial estimate

$$|a|^r - |b|^r \leq ||a| - |b|| \tag{16.2}$$

only applying to integer values of $a, b \in \mathbb{Z}$, where $r \in \mathbb{Q}_{[0,1]}$. With the help of this estimate, they obtained an integrand that no longer contains roots or rational powers of the integration variables but instead integer powers, which they then integrated against the preceding Gaussian functions. Having the KCHF procedure at hand, allowing us to integrate at least basic integrands including rational powers of the integration variable, we do not have to eliminate the rational exponent completely. Hence, while we follow the main route of the Brunnemann–Thiemann path, we do divert from it when it comes to retaining the exponent r. The new estimates that we will use in addition to or instead of the ones of Brunnemann–Thiemann, respectively, are

$$|a|^r - |b|^r \leq |a-b|^r \tag{16.3}$$
$$|a+b|^r \leq |a|^r + |b|^r \tag{16.4}$$
$$2|ab| \leq |a|^2 + |b|^2 \quad \text{and} \tag{16.5}$$
$$|a|^2 + |b|^2 \leq (|a|+|b|)^2, \tag{16.6}$$

where we can now allow $a, b, r \in \mathbb{R}$ with $0 \leq r \leq 1$. Additionally, we will later use

$$|a+C|^r - |(a-1)+C|^r \leq |a|^r - |a-1|^r + 2, \tag{16.7}$$

where $a, C, r \in \mathbb{R}$ and $0 \leq r \leq 1$. A short summary of those estimates is also provided in Appendix C for future reference.

In what follows, we often only work with the part of the integrand we perform the estimates on, which allows us to have more concise formulae. For the part of the expectation value of $\hat{q}^{i_0}_{I_0}(r)$ that contains the difference of the shifted and unshifted eigenvalues of the volume operator only, we have in the notation of [65, 66]

$$\begin{aligned} \Delta\lambda^r &:= \lambda^r\big(\{n^i_I\}\big) - \lambda^r\big(\{n^i_I + \delta^{ii_0}\delta_{II_0}\}\big) \\ &= {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}} \left(\left| \sum_{IJK} \epsilon(IJK)\epsilon_{ijk} n^i_I n^j_J n^k_K \right|^{\frac{r}{2}} - \right. \\ &\qquad \left. - \left| \sum_{IJK} \epsilon(IJK)\epsilon_{ijk} n^i_I n^j_J n^k_K + 3\sum_{JK} \epsilon(I_0JK)\epsilon_{i_0jk} n^j_J n^k_K \right|^{\frac{r}{2}} \right). \end{aligned} \tag{16.8}$$

As before, we used the shorthand notation $\sum_{IJK}$ for summing over all combinations of distinct edges e_I, e_J and e_K that meet at the vertex v. Likewise, $\sum_{JK}$ collects all edges $e_J \neq e_K$ that meet at v with I_0. We already know that integrating this expression against Gaussian functions is a cul-de-sac and we now want to proceed with using estimates. However, we saw that also with the help of KCHFs we could only integrate rather basic functions of the integration variables and rational exponents, so the estimates we use should try to simplify the structure of the terms above. We currently face rational powers of absolute values of sums of determinants and we need to get expressions that are, at best, just sums of monomials in the charges — where we would allow the exponents to still be rational. Using the estimates stated above, we obtain the chain of estimates

$$\begin{aligned}
\Delta\lambda^r &\overset{(16.3)}{\leq} {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}3^{\frac{r}{2}}\left|\sum_{JK}\epsilon(I_0JK)\epsilon_{i_0jk}n_J^jn_K^k\right|^{\frac{r}{2}}\\
&\overset{(16.4)}{\leq} {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}3^{\frac{r}{2}}\left(\sum_{JKjk}\left|\epsilon(I_0JK)\epsilon_{i_0jk}n_J^jn_K^k\right|\right)^{\frac{r}{2}}\\
&\leq {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}3^{\frac{r}{2}}\left(\sum_{JKjk}\left|n_J^jn_K^k\right|\right)^{\frac{r}{2}}\\
&\overset{(16.5)}{\leq} {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}3^{\frac{r}{2}}\left(\frac{1}{2}\sum_{JKjk}\left(\left|n_J^j\right|^2+\left|n_K^k\right|^2\right)\right)^{\frac{r}{2}}\\
&\leq {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}3^{\frac{r}{2}}\left(\frac{1}{2}3M\left(\sum_{Jj}\left|n_J^j\right|^2+\sum_{Kk}\left|n_K^k\right|^2\right)\right)^{\frac{r}{2}}\\
&\overset{(16.6)}{\leq} {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}}\left(\sum_{Jj}\left|n_J^j\right|\right)^{r}\\
&\overset{(16.4)}{\leq} {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}}\sum_{Jj}\left|n_J^j\right|^{r}.
\end{aligned}\tag{16.9}$$

Note some subtlety of the notation used above: As we applied estimate (16.4), we do no longer have a summation over j, k inside the absolute value of the second line *et seq.* — both indices appearing twice is not understood as summing over them here. We instead sum multiple absolute values with different j, k inserted. Continuing, all ϵ were estimated as 1 and we obtained a combinatorical prefactor $3M$. It originates in the empty sum we face after having applied (16.5). In the fourth line, the first term n_J^i that is summed over all J, K, j, k does not contain K or k and vice versa for the second term. While of course not all M edges necessarily meet at v — and, in fact, with two edges being fixed it would be $M-2$ maximum —, we still estimate the overall amount by M for reasons of brevity and to be able to compare our result with [66], who used M as well. The same holds for the 3 of the empty sum over the remaining (in fact one) U(1)-charge.
This expression, (16.9), is what we now need to integrate against Gaussians in the n_J^j. The equivalent part of the integrand of Brunnemann–Thiemann reads [66, eq. (C.39) therein]

$$|\Delta\lambda^r| \overset{\text{B.–T.}}{\leq} {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}9M\sum_{Jj}\left|n_J^j\right|^2 \tag{16.10}$$

and we see that we obtained a quite similar expression. However, as we already argued, Brunnemann–Thiemann wanted to replace the rational exponent r by integer ones, while we still have r. Having in mind that $0 \leq r < 1$, we can deduce the new estimate to be less rough due to $r < 2$ and $M, \left|n_J^j\right| \in \mathbb{N}_0$. Still, we were not able to preserve the initial power in the charges, $|n|^{\frac{3r}{2}}$. As we will later see and one may expect, this affects the final result and is the very reason why we will try to find more suitable estimates in Section 16.2

Continuing with the integration of (16.9), we have

$$\begin{aligned}
\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m} &\leq \frac{{\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}}}{a^{3r}\|\Psi_m\|^2} \sum_{\{n_I^i\}\in\mathbb{Z}} \mathrm{e}^{\sum_{Ii}\left(-t\left(n_I^i\right)^2+2p_I^i n_I^i\right)} \sum_{Jj}\left|n_J^j\right|^r \\
&= \frac{\xi}{\|\Psi_m\|^2} \sum_{\{N_I^i\}\in\mathbb{Z}} \int_{-\infty}^{\infty} \mathrm{d}^{3M}x_I^i \left(\frac{2\pi}{T}\right)^{3M} \mathrm{e}^{\sum_{Ii}\left(-\left(x_I^i\right)^2+\frac{2p_I^i}{T}x_I^i-\frac{2\pi\mathrm{i}N_I^i}{T}x_I^i\right)} \sum_{Jj}\frac{\left|x_J^j\right|^r}{T^r} \\
&= \frac{\xi}{\|\Psi_m\|^2}\frac{(2\pi)^{3M}\sqrt{\pi}^{3M-1}}{T^{3M+r}} \sum_{\{N_I^i\}\in\mathbb{Z}}\sum_{Jj} \mathrm{e}^{\sum_{Ii\setminus Jj}\left(\frac{p_I^i}{T}-\frac{\pi\mathrm{i}N_I^i}{T}\right)^2}\Gamma\left(\tfrac{r+1}{2}\right)\cdot \\
&\quad \cdot {}_1\mathrm{F}_1\left(\frac{r+1}{2},\frac{1}{2},\left(\frac{p_J^j}{T}-\frac{\pi\mathrm{i}N_J^j}{T}\right)^2\right),
\end{aligned} \tag{16.11}$$

where we combined all prefactors in $\xi := T^{3r}|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}}$. In the second line, we also realised that we integrate only one x_J^j over a Gaussian multiplied by the absolute value to the power of r, while all remaining ones are just of standard Gaussian form:

$$\int_{-\infty}^{\infty} \mathrm{d}x_I^i\, \mathrm{e}^{-\left(x_I^i\right)^2+\left(\frac{2p_I^i}{T}-\frac{2\pi\mathrm{i}N_I^i}{T}\right)x_I^i} = \sqrt{\pi}\,\mathrm{e}^{\left(\frac{p_I^i}{T}-\frac{\pi\mathrm{i}N_I^i}{T}\right)^2}. \tag{16.12}$$

The ones including the absolute value to the power of r result in a KCHF, just as before:

$$\int_{-\infty}^{\infty} \mathrm{d}x_J^j\, \mathrm{e}^{\left(x_J^j\right)^2+\left(\frac{2p_J^j}{T}-\frac{2\pi\mathrm{i}N_J^j}{T}\right)x_J^j}\left|x_J^j\right|^r = \Gamma\left(\tfrac{r+1}{2}\right){}_1\mathrm{F}_1\left(\frac{r+1}{2},\frac{1}{2},\left(\frac{p_J^j}{T}-\frac{\pi\mathrm{i}N_J^j}{T}\right)^2\right). \tag{16.13}$$

This is the reason why in the third line of (16.11), the product of the Gaussians does not include the one for (j, J) — symbolised by $\sum_{Ii\setminus Jj}$ — as for that we instead have the factor corresponding to the right hand side of (16.13). With this, we can perform the by now familiar follow-up steps of inserting the norm of the states,

$$\|\Psi_m\|^2 = \left(\frac{2\pi\sqrt{\pi}}{T}\right)^{3M} \mathrm{e}^{\sum_{Ii}\left(\frac{p_I^i}{T}\right)^2} \prod_{Ii}\big(1 + K^i_{t(I)}\big), \tag{16.14}$$

applying the asymptotic expansion for large arguments of the KCHF and discarding all terms $N_I^i \neq 0$, to obtain

$$\frac{\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m}}{t} \leq (16.11) \overset{t\to 0}{=} T^{3r}|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}} \sum_{Jj}\sum_{n=0}^{\infty} \frac{\left(-\frac{r}{2}\right)_n\left(\frac{1-r}{2}\right)_n}{n!}\left|p_J^j\right|^{r-2n} t^{n-r-1}. \tag{16.15}$$

We directly state the corresponding result for the important case of $r = \frac{1}{2}$, i.e. where the root of the volume operator is contained in $\hat{q}^{i_0}_{I_0}(r)$:

$$\frac{\langle \hat{q}^{i_0}_{I_0}\left(\frac{1}{2}\right)\rangle_{\Psi_m}}{t} \overset{t\to 0}{\lesssim} T^{\frac{3}{2}}|Z|^{\frac{1}{4}}(9M)^{\frac{1}{4}} \sum_{Jj}\left(\frac{\sqrt{|p_J^j|}}{\sqrt{t}^3} - \frac{1}{16}\frac{1}{\sqrt{t}\sqrt{|p_J^j|}^3} - \frac{15}{256}\frac{\sqrt{t}}{\sqrt{|p_J^j|}^7} + \mathcal{O}\left(t^{\frac{3}{2}}\right)\right), \tag{16.16}$$

with the leading order

$$\frac{\langle \hat{q}^{i_0}_{I_0}\left(\frac{1}{2}\right)\rangle_{\Psi_m}}{t} \overset{t\to 0}{\lesssim} |Z|^{\frac{1}{4}}(9M)^{\frac{1}{4}} \sum_{Jj} \frac{\sqrt{|p_J^j|}}{t^{\frac{3}{4}}} + \mathcal{O}\left(t^{\frac{1}{4}}\right). \tag{16.17}$$

We may now want to investigate the cosmological singularity, i.e. consider the limit $p \to 0$. As before, this forces us to deviate from how we proceeded from (16.11) onwards as we can no longer argue that the argument of the KCHF is large, which allowed us to apply the asymptotic expansion.[1] However, we can instead first perform a Kummer transformation according to (11.11) and then insert the definition of the KCHF in terms of a power series, (11.2), leading to

$$\frac{\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m}}{t} \overset{p_I^i = 0}{\leq} \frac{|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}}}{\sqrt{\pi}}\Gamma\left(\tfrac{r+1}{2}\right)t^{r-1} \sum_{\{N_I^i\}\in\mathbb{Z}}\sum_{Jj} \mathrm{e}^{-\sum_{Ii\setminus Jj}\frac{\pi^2}{t}\left(N_I^i\right)^2}.$$
$$\cdot\, {}_1\mathrm{F}_1\left(\frac{r+1}{2}, \frac{1}{2}, -\frac{\pi^2}{t}\left(N_J^j\right)^2\right)$$

[1]Note that we will ultimately only consider contributions with $N_I^i = 0$.

$$\begin{aligned}
&\overset{(11.11)}{=} \frac{|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}}}{\sqrt{\pi}}\Gamma\big(\tfrac{r+1}{2}\big)t^{r-1} \sum_{\{N_I^i\}\in\mathbb{Z}} \sum_{Jj} \mathrm{e}^{-\sum_{Ii}\frac{\pi^2}{t}\left(N_I^i\right)^2} \cdot \\
&\quad \cdot {}_1\mathrm{F}_1\left(-\frac{r}{2},\frac{1}{2},\frac{\pi^2}{t}\big(N_J^j\big)^2\right) \\
&\overset{(11.2)}{=} \frac{|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}}}{\sqrt{\pi}}\Gamma\big(\tfrac{r+1}{2}\big)t^{r-1} \sum_{\{N_I^i\}\in\mathbb{Z}} \sum_{Jj} \mathrm{e}^{-\sum_{Ii}\frac{\pi^2}{t}\left(N_I^i\right)^2} \cdot \\
&\quad \cdot \sum_{n=0}^{\infty} \frac{\big(-\frac{r}{2}\big)_n}{\big(\frac{1}{2}\big)_n n!}\left(\frac{\pi^2}{t}\big(N_J^j\big)^2\right)^n \\
&= \frac{|Z|^{\frac{r}{2}}(9M)^{\frac{r}{2}}}{\sqrt{\pi}}\Gamma\big(\tfrac{r+1}{2}\big)t^{r-1} \sum_{\{N_I^i\}\in\mathbb{Z}} \sum_{Jj} \mathrm{e}^{-\sum_{Ii}\frac{\pi^2}{t}\left(N_I^i\right)^2} \cdot \\
&\quad \cdot \left(1 - r\frac{\pi^2}{t}\big(N_J^j\big)^2 + \frac{2-r}{6}\frac{\pi^4}{t^2}\big(N_J^j\big)^4 + \mathcal{O}\big(t^{-3}\big)\right).
\end{aligned} \tag{16.18}$$

With there still being Gaussians in the N_I^i present, we can again consider the terms with $N_I^i = 0$ only and finally get the upper bound of the semiclassical expectation value of $\hat{q}_{I_0}^{i_0}(r)$ divided by t in both limits $p \to 0$ and $t \to 0$:

$$\frac{\langle \hat{q}_{I_0}^{i_0}(r)\rangle_{\Psi_m}}{t} \overset{p_I^i=0}{\leq} \frac{|Z|^{\frac{r}{2}}(9M)^{1+\frac{r}{2}}}{\sqrt{\pi}}\Gamma\big(\tfrac{r+1}{2}\big)t^{r-1}. \tag{16.19}$$

Choosing the volume operator itself to be contained in $\hat{q}_{I_0}^{i_0}(r)$, i.e. $r = 1$, yields a first order contributing with t^0. Still, it is not a problem at all that we do not obtain a t^0 contribution as lowest order *in general* — remember that this was not even the case in standard quantum mechanics, confer (11.36).

As a final remark on this first application of an estimative approach using KCHFs, we note that all the results (16.15), (16.16) and (16.19) did not reflect the initial exponents of the momenta. Having started with the volume operator to the power of r, i.e. $\sim n^{\frac{3r}{2}}$, using the estimates leading to (16.9) resulted in an expression $\sim n^r$ — which ultimately yielded p^r. The t-dependency, meanwhile, ended up being $t^{\frac{r}{2}-1}$ for the lowest order contribution in (16.15), changing to t^{r-1} for the limit $p \to 0$ in (16.19). This change, however, was not caused by applying additional estimates — both results come from (16.11) with only identities or (asymptotic) expansions being applied thereafter.

16.1.2 Generalisation to products of $\hat{q}^{i_k}_{I_k}$

Having introduced the estimative approach à la Brunnemann–Thiemann with KCHFs in the previous subsection, we now generalise it to products $\prod_{k=1}^{N} \hat{q}^{i_k}_{I_k}$, where k labels the specific choice of the U(1)-copy and the edge on which the holonomy acts for each operator of the product. We can then use the estimate we found for a single $\hat{q}^{i_0}_{I_0}(r)$, (16.9), to deduce the semiclassical expectation value of a product of these operators:

$$\begin{aligned}
\langle \prod_{k=1}^{N} \hat{q}^{i_k}_{I_k}(r) \rangle_{\Psi_m} &\leq \frac{{\ell_{\mathrm{P}}}^{3rN} |Z|^{\frac{rN}{2}} (9M)^{\frac{rN}{2}}}{a^{3rN} \|\Psi_m\|^2} \sum_{\{n^i_I\}\in\mathbb{Z}} \mathrm{e}^{\sum_{Ii}\left(-t\left(n^i_I\right)^2 + 2p^i_I n^i_I\right)} \left(\sum_{Jj} \left|n^j_J\right|^r\right)^N \\
&\leq \frac{T^{3rN} |Z|^{\frac{rN}{2}} (9M)^{\frac{rN}{2}}}{\sqrt{\pi}^{3M}} \sum_{\{N^i_I\}\in\mathbb{Z}} \mathrm{e}^{-\sum_{Ii} \frac{\pi^2 \left(N^i_I\right)^2}{t}} \int_{-\infty}^{\infty} \mathrm{d}^{3M} x^i_I \; \mathrm{e}^{-\sum_{Ii}\left(x^i_I - \frac{p^i_I - \pi \mathrm{i} N^i_I}{T}\right)^2} \left(\sum_{Ii} \frac{\left|x^i_I\right|^r}{T^r}\right)^N .
\end{aligned} \tag{16.20}$$

In contrast to the single $\hat{q}^{i_0}_{I_0}(r)$, we now face the sum over all the absolute values to the power of r being taken to the power of N. Hence, we have to add some more structure to tackle the remaining integrations:

$$\left(\sum_{Ii} \frac{\left|x^i_I\right|^r}{T^r}\right)^N = \frac{1}{T^{rN}} \sum_{\{n_{\mathfrak{k}}\}} c_{n_{\mathfrak{k}}} \prod_{Ii} \left|x^i_I\right|^{r n^i_{I,\mathfrak{k}}}, \tag{16.21}$$

with

$$c_{n_{\mathfrak{k}}} := \frac{N!}{\prod_{Ii} n^i_{I,\mathfrak{k}}!} = \binom{N}{n^1_{1,\mathfrak{k}}, n^2_{1,\mathfrak{k}}, \ldots, n^3_{M,\mathfrak{k}}}. \tag{16.22}$$

Via the sum $\sum_{\{n_{\mathfrak{k}}\}}$, we consider all distributions of N into non-negative integers $n^i_{I,\mathfrak{k}} \in \mathbb{N}_+$, i.e. with $\sum_{Ii} n^i_{I,\mathfrak{k}} = N$. The combinatorical prefactors are then just the multinomial coefficients $c_{n_{\mathfrak{k}}}$.

With this, all integrals that are not just of standard Gaussian type read

$$\begin{aligned}
\mathcal{I}_{n^i_{I,\mathfrak{k}}} &:= \int_{-\infty}^{\infty} \mathrm{d}x^i_I \; \mathrm{e}^{-\left(x^i_I - \frac{p^i_I - \pi \mathrm{i} N^i_I}{T}\right)^2} \left|x^i_I\right|^{r n^i_{I,\mathfrak{k}}} \\
&= \Gamma\left(\tfrac{1 + r n^i_{I,\mathfrak{k}}}{2}\right) \mathrm{e}^{-\left(\frac{p^i_I - \pi \mathrm{i} N^i_I}{T}\right)^2} {}_1\mathrm{F}_1\left(\tfrac{1 + r n^i_{I,\mathfrak{k}}}{2}, \tfrac{1}{2}, \left(\tfrac{p^i_I - \pi \mathrm{i} N^i_I}{T}\right)^2\right)
\end{aligned} \tag{16.23}$$

and we can proceed as usual — i.e. first consider the general case of $p \neq 0$ and proceed with the asymptotic expansion for large arguments of the KCHF. Note that our notation also allows to cover all the integrals of standard Gaussian type as well, just set $n^i_{I,\mathfrak{K}} = 0$. Performing all further steps such as neglecting contributions with $N^i_I \neq 0$ yields

$$\mathcal{I}_{n^i_{I,\mathfrak{K}}} \overset{t\to 0}{=} \Gamma\left(\tfrac{1}{2}\right) \frac{|p^i_I|^{rn^i_{I,\mathfrak{K}}}}{T^{rn^i_{I,\mathfrak{K}}}} \left(1 - \frac{rn^i_{I,\mathfrak{K}}\left(1 - rn^i_{I,\mathfrak{K}}\right)}{4} \frac{t}{\left(p^i_I\right)^2} + \mathcal{O}\left(t^2\right)\right) \tag{16.24}$$

and altogether we obtain

$$\begin{aligned} \langle \prod_{k=1}^{N} \hat{q}^{i_k}_{I_k}(r) \rangle_{\Psi_m} &\overset{t\to 0}{\leq} \\ &\overset{t\to 0}{\leq} T^{3rN} |Z|^{\frac{rN}{2}} (9M)^{\frac{rN}{2}} \sum_{\{n_{\mathfrak{K}}\}} \frac{c_{n_{\mathfrak{K}}}}{T^{rN}} \prod_{Ii} \frac{|p^i_I|^{rn^i_{I,\mathfrak{K}}}}{T^{rn^i_{I,\mathfrak{K}}}} \left(1 - \frac{rn^i_{I,\mathfrak{K}}\left(1 - rn^i_{I,\mathfrak{K}}\right)}{4} \frac{t}{\left(p^i_I\right)^2} + \mathcal{O}\left(t^2\right)\right) \\ &\leq t^{\frac{rN}{2}} |Z|^{\frac{rN}{2}} (9M)^{\frac{rN}{2}} (3M)^N |p_{\max}|^{rN} + \mathcal{O}\left(t^{\frac{rN}{2}+1}\right), \end{aligned} \tag{16.25}$$

where we additionally estimated all p^i_I by $p_{\max} := \max_{Ii}\{p^i_I\}$. This allowed us to combine $\prod_{Ii} |p^i_I|^{rn^i_{I,\mathfrak{K}}}$ to $p^{rN}_{\max}$ as an upper bound and to use

$$\sum_{\{n_{\mathfrak{K}}\}} c_{n_{\mathfrak{K}}} = (3M)^N \tag{16.26}$$

as there were no other dependencies of $n_{\mathfrak{K}}$ left. With additionally dividing by t^N to account for the N-fold product of the operators, the final result reads

$$\frac{\langle \prod_{k=1}^{N} \hat{q}^{i_k}_{I_k}(r) \rangle_{\Psi_m}}{t^N} \overset{t\to 0}{\leq} t^{\left(\frac{r}{2}-1\right)N} |Z|^{\frac{rN}{2}} (9M)^{\frac{rN}{2}} (3M)^N |p_{\max}|^{rN} + \mathcal{O}\left(t^{\left(\frac{r}{2}-1\right)N+1}\right). \tag{16.27}$$

Turning towards the cosmological singularity, we have to change our tactics from (16.23) onwards, just like before. With a Kummer transformation according to (11.11), we have

$$\begin{aligned} \mathcal{I}_{n^i_{I,\mathfrak{K}}} &\overset{p=0}{=} \mathrm{e}^{\frac{\pi^2\left(N^i_I\right)^2}{t}} \Gamma\left(\frac{1+rn^i_{I,\mathfrak{K}}}{2}\right) {}_1\mathrm{F}_1\left(\frac{1+rn^i_{I,\mathfrak{K}}}{2}, \frac{1}{2}, -\frac{\pi^2\left(N^i_I\right)^2}{t}\right) \\ &= \Gamma\left(\frac{1+n^i_{I,\mathfrak{K}}}{2}\right) {}_1\mathrm{F}_1\left(-\frac{rn^i_{I,\mathfrak{K}}}{2}, \frac{1}{2}, \frac{\pi^2\left(N^i_I\right)^2}{t}\right) \end{aligned} \tag{16.28}$$

and the preceding Gaussian in (16.20) tells us we can again neglect all contributions

$N_I^i \neq 0$. With inserting the defining power series (11.2) of the KCHF, we get

$$\mathrm{e}^{-\frac{\pi^2\left(N_I^i\right)^2}{t}} \cdot \mathcal{I}_{n^i_{I,\mathfrak{k}}} \overset{p=0}{=} \Gamma\left(\tfrac{1+rn^i_{I,\mathfrak{k}}}{2}\right)\mathrm{e}^{-\frac{\pi^2\left(N_I^i\right)^2}{t}}\left(1 - rn^i_{I,\mathfrak{k}}\frac{\pi^2(N_I^i)^2}{t} + \mathcal{O}\left(t^{-2}\right)\right) = \Gamma\left(\tfrac{1+rn^i_{I,\mathfrak{k}}}{2}\right). \tag{16.29}$$

We can then combine these parts for all the factors of the product to obtain

$$\langle\prod_{k=1}^{N} \hat{q}^{i_k}_{I_k}(r)\rangle_{\Psi_m} \overset{p=0}{\leq} t^{rN}(9M)^{\frac{rN}{2}}|Z|^{\frac{rN}{2}} \sum_{\{n_\mathfrak{k}\}} \frac{c_{n_k}}{\sqrt{\pi}^{3M}} \prod_{Ii} \Gamma\left(\tfrac{1+rn^i_{I,\mathfrak{k}}}{2}\right) \tag{16.30}$$

as an intermediate step towards the final result, which ultimately also considers the division by t^N:

$$\langle\frac{\prod_{k=1}^{N} \hat{q}^{i_k}_{I_k}(r)}{t^N}\rangle_{\Psi_m} \overset{p=0}{\leq} t^{(r-1)N}(9M)^{\frac{rN}{2}}|Z|^{\frac{rN}{2}} \sum_{\{n_\mathfrak{k}\}} \frac{c_{n_k}}{\sqrt{\pi}^{3M}} \prod_{Ii} \Gamma\left(\tfrac{1+rn^i_{I,\mathfrak{k}}}{2}\right). \tag{16.31}$$

With a factor $\sqrt{\pi}^{3M}$ still being present in the denominator, it may now look as if some normalisation did not work out as expected. However, this factor is (partially) compensated by all $\Gamma\left(\left(1+rn^i_{I,\mathfrak{k}}\right)/2\right)$ for which $n^i_{I,\mathfrak{k}} = 0$. What remains is a factor $\sqrt{\pi}^{\sharp(n^i_{I,\mathfrak{k}})}$, where we denote by $\sharp(n^i_{I,\mathfrak{k}})$ the number of non-zero $n^i_{I,\mathfrak{k}}$ within the respective decomposition $n_\mathfrak{k}$. This corresponds to and stems from the number of integrals that were not just of standard Gaussian type and therefore resulted in $\Gamma\left(\left(1+rn^i_{I,\mathfrak{k}}\right)/2\right)$ instead of $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$. What is more, having a fraction of a gamma function and a square root of π within our final result is nothing new, have we also seen this behaviour in (14.30) and even in (11.36) during the quantum mechanical treatment.

The Brunnemann–Thiemann path can therefore be modified by using KCHFs in order to compute semiclassical expectation values of N-fold products of the operators $\hat{q}^{i_k}_{I_k}$. This allowed us to preserve the initial exponents at least to some extent: We were able to keep them fractional and did not need to replace them by integer ones, but the estimates still altered them. Concerning the semiclassical limit $t \to 0$, we obtained the same divergence like Brunnemann–Thiemann. In what follows, we aim at improving the estimates à la Brunnemann–Thiemann we used so far and try to understand how this choice affects the final dependence on the classicality parameter and the momenta.

16.2 New estimates

From what we saw up to now, we are led to think that an improved estimate, which will turn out to recreate the correct dependency on t and p, should still be one featuring a difference in two terms — where one somehow contains the shift and the other does not. We already realised that breaking the expression down to one contribution destroys not only the exponent of the integration variables but also causes the lowest order term of the resulting power series to survive — there is no counterpart that could compensate it in the way it happened during our analytical computations of Chapter 14. Simultaneously, we have to simplify the expressions with the KCHF procedure not allowing too complex functions of the integration variables as integrand.

To recap, our starting point is

$$\lambda^r\big(\{n_I^i\}\big)-\lambda^r\big(\{n_I^i+\delta^{ii_0}\delta_{II_0}\}\big) = {\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}\left(\left|\sum_{IJK}\det\big(n_I^i n_J^j n_K^k\big)\right|^{\frac{r}{2}} - \right.$$
$$\left. - \left|\sum_{IJK}\det\Big(\big(n_I^i+\delta^{ii_0}\delta_{II_0}\big)\big(n_J^j+\delta^{ji_0}\delta_{JI_0}\big)\big(n_K^k+\delta^{ki_0}\delta_{KI_0}\big)\Big)\right|^{\frac{r}{2}}\right). \tag{16.32}$$

One possible path now is to factor out one charge after the other. For this, we can use Laplace's rule once more. To introduce the principle, we apply it to a difference of two matrices which should mimic a charge matrix and its shifted counterpart:

$$\left|\det\begin{pmatrix} a & b & c\\ d & e & f\\ g & h & i\end{pmatrix}\right|^{\frac{r}{2}} - \left|\det\begin{pmatrix} (a-1) & b & c\\ d & e & f\\ g & h & i\end{pmatrix}\right|^{\frac{r}{2}} = \left|a\det(a_-)+\widetilde{C}\right|^{\frac{r}{2}} - \left|(a-1)\det(a_-)+\widetilde{C}\right|^{\frac{r}{2}}. \tag{16.33}$$

Therein, we used $\det(a_-)$ for the minor of the matrix with respect to the element a, while $\widetilde{C} := -b\det(b_-)+c\det(c_-)$ collects all contributions that do not contain that a.

If we now think about how an estimate of the expression above should look like such that we can not only integrate it but also in a way that it still is a difference in two terms — therefore leading to a difference in two KCHFs and an elimination of the zeroth order contribution —, we realise that getting rid of $\widetilde{C}$ would yield precisely such an expression: After factoring out $\det(a_-)$, integrating over a results in a difference in two KCHFs and the remaining integration over the variables in $\det(a_-)$ can be handled via suitable substitutions. To start into this direction, we first of all rewrite

$$\left|a\det(a_-)+\widetilde{C}\right|^{\frac{r}{2}}-\left|(a-1)\det(a_-)+\widetilde{C}\right|^{\frac{r}{2}}=:(\det(a_-))^{\frac{r}{2}}\Big(|a+C|^{\frac{r}{2}}-|(a-1)+C|^{\frac{r}{2}}\Big),\tag{16.34}$$

as this provides an expression with isolated a. Applying now our new estimate (16.7),

$$|a+C|^{\frac{r}{2}}-|(a-1)+C|^{\frac{r}{2}}\leq|a|^{\frac{r}{2}}-|a-1|^{\frac{r}{2}}+2\ ,\tag{16.7}$$

on (16.32) including the previous reformulations, we obtain

$$\Delta\lambda^r\leq{\ell_{\mathrm{P}}}^{3r}|Z|^{\frac{r}{2}}\left|\sum_{JK}\epsilon(I_0JK)\epsilon_{i_0jk}n_J^jn_K^k\right|^{\frac{r}{2}}\Big[\big|n_{I_0}^{i_0}\big|^{\frac{r}{2}}-\big|n_{I_0}^{i_0}+1\big|^{\frac{r}{2}}+2\Big].\tag{16.35}$$

First, we note that our new estimate (16.7) indeed dropped the collection C of all additional contributions, but that came at a price: We had to include an additional offset +2, as can be quickly motivated by setting $a=0\wedge C=1$ in (16.7). See Appendix C for a proof of that inequality. As before, $\sum_{JK}$ stands for the sum over all edges e_J and e_K with $e_{I_0}\cap e_J\cap e_K=v\wedge J,K\neq I_0\wedge J\neq K$, i.e. it collects all minors of the charge matrices containing $n_{I_0}^{i_0}$ with respect to this charge. In that sense, the $\det(a_-)$ from before became a sum over those terms. Accordingly, the offset C collects all remaining terms of the Laplace expansions and those determinants of charge matrices that are independent of $n_{I_0}^{i_0}$.

With (16.35) above, we now do have an expression at hand that is integrable against the Gaussian prefactor after a previous Poisson resummation. Performing the latter after having inserted the estimate (16.35) into (16.1), the follow-up integration over $x_{I_0}^{i_0}$ results in

$$\begin{aligned}&\langle\hat{q}_{I_0}^{i_0}(r)\rangle_{\Psi_m}\leq\\&\leq\frac{T^{3r}|Z|^{\frac{r}{2}}}{\sqrt{\pi}^{3M}}\sum_{\{N_I^i\}\in\mathbb{Z}}\mathrm{e}^{-\sum_{Ii}\left(\frac{2\pi\mathrm{i}p_I^iN_I^i}{t}+\frac{\pi^2\left(N_I^i\right)^2}{t}\right)}\int\limits_{-\infty}^{\infty}\mathrm{d}^{3M-1}x_{I\setminus I_0}^{i\setminus i_0}\ \mathrm{e}^{-\sum_{Ii\setminus I_0i_0}\left(x_I^i-\frac{p_I^i-\pi\mathrm{i}N_I^i}{T}\right)^2}\cdot\\&\cdot\left|\sum_{JK}\epsilon(I_0JK)\epsilon_{i_0jk}x_J^jx_K^k\right|^{\frac{r}{2}}T^{-r}\left[T^{-\frac{r}{2}}\Gamma\big(\tfrac{r+2}{4}\big)\,{}_1\mathrm{F}_1\left(-\frac{r}{4},\frac{1}{2},-\left(\frac{p_{I_0}^{i_0}-\pi\mathrm{i}N_{I_0}^{i_0}}{T}\right)^2\right)-\right.\\&\left.-T^{-\frac{r}{2}}\Gamma\big(\tfrac{r+2}{4}\big)\,{}_1\mathrm{F}_1\left(-\frac{r}{4},\frac{1}{2},-\left(\frac{p_{I_0}^{i_0}+T^2-\pi\mathrm{i}N_{I_0}^{i_0}}{T}\right)^2\right)+2\sqrt{\pi}\right].\end{aligned}\tag{16.36}$$

We kept the basic structure of the previous inequality (16.35) so the terms in the respective square brackets correspond to each other. Continuing with the remaining integrals, we notice that the sum over all minors with respect to $x^{i_0}_{I_0}$ makes further integrations unfeasible so far. We therefore use the previously introduced inequality

$$|a+b|^r \leq |a|^r + |b|^r \quad (\text{where } a,b,r \in \mathbb{R} \text{ and } 0 \leq r \leq 1) \tag{16.4}$$

to further estimate the expression above via

$$\begin{aligned} \left|\sum_{JK} \epsilon(I_0JK)\epsilon_{i_0jk}x^j_J x^k_K\right|^{\frac{r}{2}} &\leq \sum_{JKjk} \left|\epsilon(I_0JK)\epsilon_{i_0jk}x^j_J x^k_K\right|^{\frac{r}{2}} \\ &= \sum_{JKjk} \left|x^j_J\right|^{\frac{r}{2}} \left|x^k_K\right|^{\frac{r}{2}}. \end{aligned} \tag{16.37}$$

Note that the estimate caused the sum over J,K to happen outside the absolute value and, accordingly, there is no additional summation over J,K inside the absolute value — regardless of their double appearance therein. However, we still consider only distinct $J,K \neq I_0$ and the same holds for j,k,i_0. With that, we have

$$\begin{aligned} &\int\limits_{-\infty}^{\infty} \mathrm{d}^{3M-1}x^{i\setminus i_0}_{I\setminus I_0}\ \mathrm{e}^{-\sum_{Ii\setminus I_0i_0}\left(x^i_I - \frac{p^i_I - \pi\mathrm{i}N^i_I}{T}\right)^2} \sum_{JKjk} \left|x^j_J\right|^{\frac{r}{2}} \left|x^k_K\right|^{\frac{r}{2}} = \\ &= \sqrt{\pi}^{3M-3}\,\Gamma^2\!\left(\tfrac{r+2}{4}\right) \sum_{JKjk} {}_1\mathrm{F}_1\!\left(-\frac{r}{4}, \frac{1}{2}, -\left(\frac{p^j_J - \pi\mathrm{i}N^j_J}{T}\right)^2\right) {}_1\mathrm{F}_1\!\left(-\frac{r}{4}, \frac{1}{2}, -\left(\frac{p^k_K - \pi\mathrm{i}N^k_K}{T}\right)^2\right) \end{aligned} \tag{16.38}$$

for the remaining integrals. The exponent $3M-3$ of the square root of π is due to two of the $3M-1$ many integrations resulting in a KCHF, which — in some sense — include those normalisation terms. The two Gamma functions, of course, also stem from these two integrations.

Combining all estimates and integrations, we face

$$\begin{aligned} &\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m} \leq \\ &\leq \frac{T^{3r}|Z|^{\frac{r}{2}}T^{-\frac{3r}{2}}}{\sqrt{\pi}^3} \sum_{\left\{N^i_I\right\}\in\mathbb{Z}} \mathrm{e}^{-\sum_{Ii}\left(\frac{2\pi\mathrm{i}p^i_I N^i_I}{t} + \frac{\pi^2\left(N^i_I\right)^2}{t}\right)} \Gamma^3\!\left(\tfrac{r+2}{4}\right) \left[{}_1\mathrm{F}_1\!\left(-\tfrac{r}{4}, \tfrac{1}{2}, -\left(\tfrac{p^{i_0}_{I_0} - \pi\mathrm{i}N^{i_0}_{I_0}}{T}\right)^2\right) - \right. \end{aligned}$$

$$- {}_1\mathrm{F}_1\left(-\tfrac{r}{4}, \tfrac{1}{2}, -\left(\tfrac{p_{I_0}^{i_0}+T^2-\pi\mathrm{i}N_{I_0}^{i_0}}{T}\right)^2\right) + 2\Gamma^{-1}\left(\tfrac{r+2}{4}\right)T^{\frac{r}{2}}\sqrt{\pi}\Bigg]\cdot$$

$$\cdot \sum_{JKjk} {}_1\mathrm{F}_1\left(-\tfrac{r}{4}, \tfrac{1}{2}, -\left(\tfrac{p_J^j-\pi\mathrm{i}N_J^j}{T}\right)^2\right){}_1\mathrm{F}_1\left(-\tfrac{r}{4}, \tfrac{1}{2}, -\left(\tfrac{p_K^k-\pi\mathrm{i}N_K^k}{T}\right)^2\right) , \tag{16.39}$$

on which we may now perform the asymptotic expansion for large arguments of (all) the KCHFs. *As usual*, only the contributions $N_I^i = 0$ will not vanish for $T \to 0$ and only one series per asymptotic expansion is not damped by a preceding Gaussian function. Including also the division by t in order to compare the result with the classical Poisson bracket, we find the upper bound

$$\begin{aligned}\frac{\langle \hat{q}_{I_0}^{i_0}(r)\rangle_{\Psi_m}}{t} \lesssim T^{3r}|Z|^{\frac{r}{2}}T^{-\frac{3r}{2}-2}\Bigg[\left|\frac{p_{I_0}^{i_0}}{T}\right|^{\frac{r}{2}}\sum_{s=0}^{\infty}\frac{\left(-\frac{r}{4}\right)_s\left(\frac{2-r}{4}\right)_s}{s!}\left(\frac{p_{I_0}^{i_0}}{T}\right)^{-2s} - \\ -\left|\frac{p_{I_0}^{i_0}+T^2}{T}\right|^{\frac{r}{2}}\sum_{s=0}^{\infty}\frac{\left(-\frac{r}{4}\right)_s\left(\frac{2-r}{4}\right)_s}{s!}\left(\frac{p_{I_0}^{i_0}+T^2}{T}\right)^{-2s} + 2T^{\frac{r}{2}}\Bigg]\cdot \\ \cdot\sum_{JKjk}\left(\left|\frac{p_J^j}{T}\right|^{\frac{r}{2}}\sum_{s=0}^{\infty}\frac{\left(-\frac{r}{4}\right)_s\left(\frac{2-r}{4}\right)_s}{s!}\left(\frac{p_J^j}{T}\right)^{-2s}\right)\left(\left|\frac{p_K^k}{T}\right|^{\frac{r}{2}}\sum_{s=0}^{\infty}\frac{\left(-\frac{r}{4}\right)_s\left(\frac{2-r}{4}\right)_s}{s!}\left(\frac{p_K^k}{T}\right)^{-2s}\right)\end{aligned} \tag{16.40}$$

for an arbitrary graph consisting of M edges. For the lowest order contributions up to $s = 1$, we realise that the zeroth order contributions of the sums inside the square bracket annul each other and with defining the maximum p as $|p_{\max}| = \max_{i\neq i_0, I\neq I_0}(\{|p_I^i|\})$, we have

$$\begin{aligned}\frac{\langle \hat{q}_{I_0}^{i_0}(r)\rangle_{\Psi_m}}{t} &\lesssim |Z|^{\frac{r}{2}}T^{\frac{3r}{2}-2}\Big[2T^{\frac{r}{2}} - \frac{r}{2}\operatorname{sgn} p_{I_0}^{i_0}\left|p_{I_0}^{i_0}\right|^{\frac{r}{2}-1}T^{2-\frac{r}{2}} + \mathcal{O}\big(T^{4-\frac{r}{2}}\big)\Big]\cdot \\ &\cdot\sum_{JKjk}\left(\left|p_J^j p_K^k\right|^{\frac{r}{2}}T^{-r} - r(2-r)\frac{\left(p_J^j\right)^2+\left(p_K^k\right)^2}{16\left(p_J^j\right)^2\left(p_K^k\right)^2}\left|p_J^j p_K^k\right|^{\frac{r}{2}}T^{2-r} + \mathcal{O}\big(T^{4-r}\big)\right) \\ &\lesssim |Z|^{\frac{r}{2}}2M\left(2|p_{\max}|^r t^{\frac{r}{2}-1} - \frac{r}{2}|p_{\max}|^r\operatorname{sgn} p_{I_0}^{i_0}\left|p_{I_0}^{i_0}\right|^{\frac{r}{2}-1}t^0 - \frac{r(2-r)}{4}|p_{\max}|^{r-2}t^{\frac{r}{2}}\right) + \mathcal{O}\big(t^1\big).\end{aligned} \tag{16.41}$$

Note that the introduction of $p_{\max}$ requires $p_{\max}$ to increase no faster than t approaches 0 as otherwise the order of the contributions would change. As a last step, we used $2M$ as an estimate of the sum over the remaining edges and U(1)-copies.

Taking a closer look at the new results above, we see that also these diverge for $t \to 0$ — the reason being the offset $+2T^{\frac{r}{2}}$ from our new estimate (16.35). We aimed to obtain an estimate that in the end leads to an expression that is still a difference in two KCHFs — which causes the zeroth order contributions to vanish. However, we could not entirely get this but had to include the bespoke offset $+2$. The lowest order contribution then indeed is the contribution of this offset, $2T^{\frac{r}{2}}$, multiplied with the lowest order contribution of the second line of (16.41). Otherwise, had we not to include this offset, the lowest order contribution would indeed be the t^0-term that on top of that also features the expected p-dependency: Having in mind the differentiation-like action of the Poisson bracket, we expect the exponent $\frac{r}{2}$ of the momentum $p^{i_0}_{I_0}$ to get decreased by one while also causing the numerical prefactor $\frac{r}{2}$. The other two momenta are not affected and combine to an overall p^r-dependency. This is precisely what the t^0-term above looks like.

If we now consider the limit $p \to 0$, we can again not use the asymptotic expansion for large arguments of the KCHF and have to deviate from our previous path from (16.39) onwards. As before, we first of all set $p = 0$ in (16.39). Due to the Gaussian prefactors, we can again only consider the contributions with $N^i_I = 0$. With that, most KCHFs reduce to ${}_1\mathrm{F}_1(a, b, 0) \equiv 1$, while the one that contains the shift directly yields a power series in t. We can then estimate the empty sum via $\sum_{JKjk} 1 \leq (3M)^2$ to obtain the upper bound in the limit $p \to 0$:

$$\frac{\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m}}{t} \overset{p^i_I=0}{\leq} \frac{|Z|^{\frac{r}{2}}(3M)^2}{\sqrt{\pi}^3}\Gamma^3\left(\tfrac{r+2}{4}\right)\left(\frac{2\sqrt{\pi}}{\Gamma\left(\frac{r+2}{4}\right)}t^{r-1} + \frac{r}{2}t^{\frac{3r}{4}} + \mathcal{O}\left(t^{1+\frac{3r}{4}}\right)\right). \qquad (16.42)$$

The lowest order contribution can again be linked to the offset $+2$ of our new estimate (16.35). With that, we realise that we ended up having the same t-dependencies as in Subsection 16.1.1 for both the general case and when considering $p = 0$. Accordingly, we also obtain a diverging expression when additionally taking the semiclassical limit $t \to 0$.

16.2.1 Finding them

All the estimates we used up to now made us end up with results of undesired dependencies in p or t — or both. They allowed us to integrate the thereby obtained expressions as these were simply Gaussians multiplied by absolute values of the integration variables to the power of r. However, we saw that we can in fact also compute integrals were the integrand are Gaussians and the absolute value of a determinant to the power of r — we do not actually need to reduce it to isolated x_I^i in the absolute values. So all we need to get rid of is the *sum* of determinants within the absolute value, which we can achieve via estimates as well. For this, we assume there are N charge matrices $\mathcal{N}_\mathfrak{n}$ that include the charge n_I^i, to which we assign the shift:[2]

$$\left|\sum_{\mathfrak{n}=1}^{N} \det \mathcal{N}_\mathfrak{n} + C\right|^{\frac{r}{2}} - \left|\sum_{\mathfrak{n}=1}^{N} \det \widetilde{\mathcal{N}}_\mathfrak{n} + C\right|^{\frac{r}{2}} \leq \left|\sum_{\mathfrak{n}=1}^{N} \Big(\det \mathcal{N}_\mathfrak{n} - \det \widetilde{\mathcal{N}}_\mathfrak{n}\Big)\right|^{\frac{r}{2}} . \tag{16.43}$$

The charge matrices $\widetilde{\mathcal{N}}_\mathfrak{n}$ correspond to the normal charge matrices $\mathcal{N}_\mathfrak{n}$ but include the shift in the element n_1^1. C then collects all remaining determinants and vanishes via the application of (16.3). We continue with a Laplace expansion along the three charges n_1^i of edge 1:

$$\begin{aligned}\left|\sum_{\mathfrak{n}=1}^{N} \Big(\det \mathcal{N}_\mathfrak{n} - \det \widetilde{\mathcal{N}}_\mathfrak{n}\Big)\right|^{\frac{r}{2}} &= \Bigg|\sum_{\mathfrak{n}=1}^{N} \big(n_1^1 \Delta_1^1(\mathcal{N}_\mathfrak{n})\big) - n_1^2 \Delta_1^2(\mathcal{N}_\mathfrak{n}) + n_1^3 \Delta_1^3(\mathcal{N}_\mathfrak{n}) - \\ &\qquad - \big(n_1^1 + 1\big)\Delta_1^1(\mathcal{N}_\mathfrak{n}) + n_1^2 \Delta_1^2(\mathcal{N}_\mathfrak{n}) - n_1^3 \Delta_1^3(\mathcal{N}_\mathfrak{n})\big)\Bigg|^{\frac{r}{2}} \\ &= \left|\sum_{\mathfrak{n}=1}^{N} \Delta_1^1(\mathcal{N}_\mathfrak{n})\right|^{\frac{r}{2}} \equiv \left|\sum_{IJ} \det \begin{pmatrix} n_I^2 & n_I^3 \\ n_J^2 & n_J^3 \end{pmatrix}\right|^{\frac{r}{2}} \leq \sum_{IJ} \left|\det \begin{pmatrix} n_I^2 & n_I^3 \\ n_J^2 & n_J^3 \end{pmatrix}\right|^{\frac{r}{2}} .\end{aligned} \tag{16.44}$$

Note that we again abbreviated the sum over all edges $e_I \neq e_J$ that meet e_1 at v with $\sum_{IJ}$ and the minor of the charge matrix $\mathcal{N}_\mathfrak{n}$ with respect to n_I^i as $\Delta_i^i(\mathcal{N}_\mathfrak{n})$:

$$\det \mathcal{N}_\mathfrak{n} = \det \begin{pmatrix} n_1^1 & n_1^2 & n_1^3 \\ n_I^1 & \boxed{\begin{matrix} n_I^2 & n_I^3 \\ n_J^2 & n_J^3 \end{matrix}} \\ n_J^1 & & \end{pmatrix} \leftarrow \Delta_1^1(\mathcal{N}_\mathfrak{n}) \; . \tag{16.45}$$

The most important aspect now is that we estimated the difference of two terms that are fractional powers by the fractional power of a difference of two terms. As many contributions of these two terms were the same, we are left with only the sum over all minors of the charge matrices with respect to the shifted charge. To get an integrable expression, we then applied (16.4) to cast the fractional power of a sum into the sum of

[2]As before, this can be done without loss of generality as we work with determinants, allowing us to reshuffle the matrix accordingly.

fractional powers. We now need to integrate these against the Gaussian functions. Out of these $3M$ many integrals, $3M-4$ many are not over integration variables that are also contained in the minor of the determinant. These integrals therefore are of standard Gaussian type, resulting in $\sqrt{\pi}$. Recap that during our analytical integration of the basic building block, we had to compute all $3M = 9$ many non-Gaussian-type integrals, as we did not just face the minor of the charge matrix but the whole determinant (confer Section 14.2 and Appendix B).

Applying now the Poisson resummation formula, we have with $s \coloneqq \frac{r}{2}$:

$$
\begin{aligned}
\langle \hat{q}_1^1(r) \rangle_{\Psi_m} \leq & \left(\frac{T}{2\pi\sqrt{\pi}}\right)^{3M} \mathrm{e}^{-\sum_{iI}\left(\frac{p_i^i}{T}\right)^2} \frac{\ell_{\mathrm{P}}{}^{6s}|Z|^s}{a^{6s}\prod_i(1+K^i)} \left(\frac{2\pi}{T}\right)^{3M} \sum_{\{N_I^i\}\in\mathbb{Z}} \mathrm{e}^{\sum_{iI}\left(\frac{p_I^i-\pi\mathrm{i}N_I^i}{T}\right)^2} \cdot \\
& \cdot \int\limits_{-\infty}^{\infty} \mathrm{d}^{3M}x_I^i \; \mathrm{e}^{-\sum_{iI}\left(x_I^i-\frac{p_I^i-\pi\mathrm{i}N_I^i}{T}\right)^2} \frac{1}{T^{2s}} \sum_{IJ} \left|x_I^2x_J^3 - x_I^3x_J^2\right|^s \\
= & \frac{T^{4s}|Z|^s}{\sqrt{\pi}^4\prod_i(1+K^i)} \sum_{\{N_I^i\}\in\mathbb{Z}} \mathrm{e}^{-\sum_{iI}\left(\frac{2\pi\mathrm{i}p_I^iN_I^i}{T^2}+\frac{\pi^2\left(N_I^i\right)^2}{T^2}\right)} \cdot \\
& \cdot \sum_{IJ} \int\limits_{-\infty}^{\infty} \mathrm{d}x_I^2 \int\limits_{-\infty}^{\infty} \mathrm{d}x_I^3 \int\limits_{-\infty}^{\infty} \mathrm{d}x_J^2 \int\limits_{-\infty}^{\infty} \mathrm{d}x_J^3 \; \mathrm{e}^{-\sum_{\substack{k=2,3\\K=I,J}}\left(x_K^k-\frac{p_K^k-\pi\mathrm{i}N_K^k}{T}\right)^2} \left|x_I^2x_J^3 - x_I^3x_J^2\right|^s .
\end{aligned}
\tag{16.46}
$$

The determinant-like part of the integrand can then be substituted along the line of our rigorous treatment of the basic building blocks in Section 14.2:

$$
\tilde{x}_I^2 \coloneqq x_I^2x_J^3 - x_I^3x_J^2 \tag{16.47}
$$

$$
\mathrm{d}\tilde{x}_I^2 = \left|x_J^3\right| \mathrm{d}x_I^2 \, . \tag{16.48}
$$

This leads us to

$$
\begin{aligned}
& \int\limits_{-\infty}^{\infty} \mathrm{d}\tilde{x}_I^2 \; \mathrm{e}^{-\left(\frac{\tilde{x}_I^2}{x_J^3}+\frac{x_I^3x_J^2}{x_J^3}-\frac{p_I^2-\pi\mathrm{i}N_I^2}{T}\right)^2} \frac{|\tilde{x}_I^2|^s}{|x_J^3|} = \\
& = \Gamma\!\left(\tfrac{1+r}{2}\right)\left|x_J^3\right|^s \mathrm{e}^{-\left(\frac{x_I^3x_J^2}{x_J^3}-\frac{p_I^2-\pi\mathrm{i}N_I^2}{T}\right)^2} {}_1\mathrm{F}_1\!\left(\frac{1+s}{2},\frac{1}{2},\left(\frac{x_I^3x_J^2}{x_J^3}-\frac{p_I^2-\pi\mathrm{i}N_I^2}{T}\right)^2\right)
\end{aligned}
$$

$$\approx \Gamma\big(\tfrac{1}{2}\big)\big|x_J^3\big|^s \left|\frac{x_I^3 x_J^2}{x_J^3} - \frac{p_I^2}{T}\right|^s \left(1 - \frac{s(1-s)}{4}\left(\frac{x_I^3 x_J^2}{x_J^3} - \frac{p_I^2}{T}\right)^{-2} + \mathcal{O}\big(T^3\big)\right)$$

$$\approx \Gamma\big(\tfrac{1}{2}\big)\left|x_I^3 x_J^2 - \frac{p_I^2}{T} x_J^3\right|^s \underbrace{\left(1 - \frac{s(1-s)}{4}\frac{T^2}{\big(p_I^2\big)^2} + \mathcal{O}\big(T^3\big)\right)}_{=:\mathcal{T}} \tag{16.49}$$

via (11.20) & (11.18) for the $\tilde{x}_I^2$-integration. Therein, we again only considered the contribution $N_I^2 = 0$, with all non-zero contributions being exponentially damped by the preceding Gaussian. Next, we substitute

$$\tilde{x}_J^3 := \frac{p_I^2}{T} x_J^3 - x_I^3 x_J^2 \tag{16.50}$$

$$\mathrm{d}\tilde{x}_J^3 = \left|\frac{p_I^2}{T}\right| \mathrm{d}x_J^3 \tag{16.51}$$

and solve in a similar fashion the $\tilde{x}_J^3$-integration according to

$$\Gamma\big(\tfrac{1}{2}\big)\mathcal{T}\int_{-\infty}^{\infty} \mathrm{d}\tilde{x}_J^3\ \mathrm{e}^{-\left(\frac{\tilde{x}_J^3}{p_I^2/T} + \frac{x_I^3 x_J^2}{p_I^2/T} - \frac{p_J^3 - \pi \mathrm{i} N_J^3}{T}\right)^2} \left|\frac{T}{p_I^2}\right| \big|\tilde{x}_J^3\big|^s =$$

$$= \Gamma\big(\tfrac{1}{2}\big)\mathcal{T}\,\Gamma\big(\tfrac{1+r}{2}\big)\left|\frac{p_I^2}{T}\right|^s \mathrm{e}^{-\left(\frac{x_I^3 x_J^2}{p_I^2/T} - \frac{p_J^3 - \pi \mathrm{i} N_J^3}{T}\right)^2} {}_1\mathrm{F}_1\left(\frac{1+s}{2}, \frac{1}{2}, \left(\frac{x_I^3 x_J^2}{p_I^2/T} - \frac{p_J^3 - \pi \mathrm{i} N_J^3}{T}\right)^2\right)$$

$$\approx \Gamma\big(\tfrac{1}{2}\big)^2 \mathcal{T}\left|\frac{p_I^2}{T}\right|^s \left|\frac{x_I^3 x_J^2}{p_I^2/T} - \frac{p_J^3}{T}\right|^s \left(1 - \frac{s(1-s)}{4}\left(\frac{x_I^3 x_J^2}{p_I^2/T} - \frac{p_J^3}{T}\right)^{-2} + \mathcal{O}\big(T^3\big)\right)$$

$$\approx \Gamma\big(\tfrac{1}{2}\big)^2 \mathcal{T}\left|x_I^3 x_J^2 - \frac{p_I^2 p_J^3}{T^2}\right|^s \underbrace{\left(1 - \frac{s(1-s)}{4}\frac{T^2}{\big(p_J^3\big)^2} + \mathcal{O}\big(T^3\big)\right)}_{=:\mathcal{T}'}\ . \tag{16.52}$$

We may then proceed with the $\tilde{x}_J^3$-integration, where we first substitute

$$\tilde{x}_I^3 := x_I^3 x_J^2 - \frac{p_I^2 p_J^3}{T^2} \tag{16.53}$$

$$\mathrm{d}\tilde{x}_I^3 = \big|x_J^2\big|\, \mathrm{d}x_I^3 \tag{16.54}$$

and subsequently find

$$\Gamma\big(\tfrac{1}{2}\big)^2 \mathcal{T}\mathcal{T}' \int_{-\infty}^{\infty} \mathrm{d}\tilde{x}_I^3 \; \mathrm{e}^{-\left(\frac{\tilde{x}_I^3}{x_J^2} + \frac{p_I^2 p_J^3}{T^2 x_J^2} - \frac{p_I^3 - \pi \mathrm{i} N_I^3}{T}\right)^2} \frac{|\tilde{x}_I^3|^s}{|x_J^2|} =$$

$$= \Gamma\big(\tfrac{1}{2}\big)^2 \mathcal{T}\mathcal{T}' \Gamma\big(\tfrac{1+r}{2}\big) \big|x_J^2\big|^s \; \mathrm{e}^{-\left(\frac{p_I^2 p_J^3}{T^2 x_J^2} - \frac{p_I^3 - \pi \mathrm{i} N_I^3}{T}\right)^2} {}_1\mathrm{F}_1\left(\frac{1+s}{2}, \frac{1}{2}, \left(\frac{p_I^2 p_J^3}{T^2 x_J^2} - \frac{p_I^3 - \pi \mathrm{i} N_I^3}{T}\right)^2\right)$$

$$\approx \Gamma\big(\tfrac{1}{2}\big)^3 \mathcal{T}\mathcal{T}' \left|\frac{p_I^2 p_J^3}{T^2} - \frac{p_I^3}{T} x_J^2\right|^s \left(1 - \frac{s(1-s)}{4}\left(\frac{p_I^2 p_J^3}{T^2 x_J^2} - \frac{p_I^3}{T}\right)^{-2} + \mathcal{O}\big(T^5\big)\right)$$

$$\approx \Gamma\big(\tfrac{1}{2}\big)^3 \mathcal{T}\mathcal{T}' \left|\frac{p_I^2 p_J^3}{T^2} - \frac{p_I^3}{T} x_J^2\right|^s \left(1 - \frac{s(1-s)}{4} \frac{\big(x_J^2\big)^2 T^4}{\big(p_I^2 p_J^3\big)^2} + \mathcal{O}\big(T^5\big)\right). \tag{16.55}$$

Now, the last integration will be different as the first non-constant term of the Taylor series in T is not independent of the remaining integration variable. We faced a similar situation during our integration of the basic building block and we therefore continue analogously by first setting

$$\tilde{x}_J^2 := \frac{p_I^3}{T} x_J^2 - \frac{p_I^2 p_J^3}{T^2} \tag{16.56}$$

$$\mathrm{d}\tilde{x}_J^2 = \left|\frac{p_I^3}{T}\right| \mathrm{d}x_J^2 \tag{16.57}$$

and then using (B.33) to get

$$\Gamma\big(\tfrac{1}{2}\big)^3 \mathcal{T}\mathcal{T}' \int_{-\infty}^{\infty} \mathrm{d}\tilde{x}_J^2 \left|\frac{T}{p_I^3}\right| \mathrm{e}^{-\left(\frac{\tilde{x}_J^2}{p_I^3/T} + \frac{p_I^2 p_J^3}{T^2 p_I^3/T} - \frac{p_J^2 - \pi \mathrm{i} N_J^2}{T}\right)^2} \big|\tilde{x}_J^2\big|^s \cdot$$

$$\cdot \left(1 - \frac{s(1-s)}{4} \frac{T^4}{\big(p_I^2 p_J^3\big)^2} \left(\frac{\tilde{x}_J^2}{p_I^3/T} + \frac{p_I^2 p_J^3}{T^2 p_I^3/T}\right)^2\right) =$$

$$= \Gamma\big(\tfrac{1}{2}\big)^3 \mathcal{T}\mathcal{T}' \Gamma\big(\tfrac{1+r}{2}\big) \left|\frac{p_I^3}{T}\right|^2 \frac{\mathrm{e}^{-\left(\frac{\Delta_1^1(p)}{p_I^3 T}\right)^2}}{8\big(p_I^2 p_I^3 p_J^3\big)^2} \cdot$$

$$\cdot \Bigg[2\big(p_I^2 p_J^3\big)^2 \Big(4\big(p_I^3\big)^2 - s(1-s)T^2\Big) {}_1\mathrm{F}_1\left(\frac{1+s}{2}, \frac{1}{2}, \left(\frac{\Delta_1^1(p)}{p_I^3 T}\right)^2\right) +$$

$$+ s\big(1-s^2\big)T^2 \left(\big(p_I^3 T\big)^2 {}_1\mathrm{F}_1\left(\frac{3+s}{2}, \frac{1}{2}, \left(\frac{\Delta_1^1(p)}{p_I^3 T}\right)^2\right)\right)$$

$$-4\Delta_1^1(p)\, p_I^2 p_J^3\, {}_1\mathrm{F}_1\left(\frac{3+s}{2}, \frac{3}{2}, \left(\frac{\Delta_1^1(p)}{p_I^3 T}\right)^2\right)\Bigg)\Bigg]$$

$$\approx \Gamma\big(\tfrac{1}{2}\big)^4 \mathcal{T}\mathcal{T}' \left|\frac{\Delta_1^1(p)}{T^2}\right|^s \left(1 - \frac{s(1-s)}{4}\left(\frac{p_I^3}{\Delta_1^1(p)}\right)^2 T^2 - \frac{s(1-s)}{4}\left(\frac{p_J^2}{p_I^2 p_J^3}\right)^2 T^2 + \mathcal{O}\big(T^3\big)\right) . \tag{16.58}$$

In accordance with the minor of the charge matrices, we defined the minors of the momentum matrix with respect to p_1^1 as

$$\Delta_1^1(p) \coloneqq p_I^2 p_J^3 - p_I^3 p_J^2 \ . \tag{16.59}$$

Note that we refrained from including the indices I, J due to reasons of clearer formulae and we just keep in mind that there is not just one such minor. As the penultimate step, we insert all the previous results into (16.46), multiply the expansion with both $\mathcal{T}$ and $\mathcal{T}'$ while keeping terms of the order T^2 and obtain

$$\begin{aligned}\langle \hat{q}_1^1(r)\rangle_{\Psi_m} &\leq \frac{T^{4s}|Z|^s}{\prod_i (1+K^i)} \sum_{IJ} \left|\frac{\Delta_1^1(p)}{T^2}\right|^s \left(1 - \frac{s(1-s)}{4}\mathcal{P}_{IJ} T^2 + \mathcal{O}\big(T^3\big)\right) \\ &= \frac{|Z|^s}{\prod_i (1+K^i)} \sum_{IJ} \big|\Delta_1^1(p)\big|^s T^{2s} \left(1 - \frac{s(1-s)}{4}\mathcal{P}_{IJ} T^2 + \mathcal{O}\big(T^3\big)\right).\end{aligned} \tag{16.60}$$

Therein, we collected all p-dependent parts of the T^2-contribution of the series in

$$\mathcal{P}_{IJ} \coloneqq \frac{\big(p_I^2 p_I^3 p_J^3\big)^2 + \big(\Delta_1^1(p)\big)^2 \Big(\big(p_I^2\big)^2 + \big(p_J^2\big)^2 + \big(p_J^3\big)^2\Big)}{\big(\Delta_1^1(p)\, p_I^2 p_J^3\big)^2}. \tag{16.61}$$

We finally divide by t to get the lowest order contribution

$$\frac{\langle \hat{q}_1^1(r)\rangle_{\Psi_m}}{t} \lesssim |Z|^{\frac{r}{2}} \sum_{IJ} \big|\Delta_1^1(p)\big|^{\frac{r}{2}} t^{\frac{r}{2}-1} + \mathcal{O}\big(t^{\frac{r}{2}}\big), \tag{16.62}$$

which for the general case of the shift happening in entry (i_0, I_0) reads

$$\frac{\langle \hat{q}_{I_0}^{i_0}(r)\rangle_{\Psi_m}}{t} \lesssim |Z|^{\frac{r}{2}} \sum_{IJ} \big|\Delta_{I_0}^{i_0}(p)\big|^{\frac{r}{2}} t^{\frac{r}{2}-1} + \mathcal{O}\big(t^{\frac{r}{2}}\big). \tag{16.63}$$

Analysing the p-dependency, we first recap that our starting point was an expression $\sim p^{3s} = p^{3r/2}$, while we ultimately arrived at one that is $\sim \Delta_{I_0}^{i_0}(p)^{\frac{r}{2}}$, i.e. $\sim p^r$. From the derivative-like action of the Poisson bracket, we expected the lowest order to contribute with $\sim p^{3r/2-1}$. However, this lowest order term is also expected to be $\sim t^0$, which is not per se true for the result above — and we can even face a negative exponent of t, for example if we consider the important case of $r = \frac{1}{2}$ when the square root of the volume operator is part of $\hat{q}^{i_0}_{I_0}(r)$.

Like during our previous calculation of semiclassical expectation values of $\hat{q}^{i_0}_{I_0}(r)$, we have to proceed differently if being interested in the cosmological singularity $p = 0$ as we notice that the asymptotic expansion for large arguments of the KCHF during (16.52) is not applicable in this case. We therefore need to apply further estimates on the determinant-like part of the integrand in (16.46) and we can deduce that doing so will lead us to a similar expression as (14.31) or (16.19) up to numerical factors.

16.2.2 Conditions for new estimates

We now summarise which different estimative routes we took so far. In Subsection 16.1.1, we presented a chain of estimates that is similar to the one Brunnemann and Thiemann chose in [66], just that we did not perform the step of replacing the fractional powers with integer ones. Next, in Section 16.2, we aimed at keeping the difference in the two absolute values when applying estimates. While we found a respective estimate that also made the expression integrable, we had to include a t-independent offset which then also altered the p- and t-dependency. Subsection 16.2.1 then was about estimates that do not yield absolute values of the plain charges but only let us replace the absolute value of a sum of determinants by a sum of the absolute values of determinants: From our rigorous integration of the basic building block in Section 14.2 and Appendix B, we know that we can in fact integrate single determinants within an absolute value to the power of r. Yet, the estimate went too far as it automatically reduced the expression to the minor of the determinant — and resulted in a single KCHF only.

We can now state some observations on properties of estimates as we analysed different approaches in the previous subsections. Our first attempts, along the line of Brunnemann and Thiemann [66], lead us to the conclusion that any estimate(s) we use should still result in

1. having a difference in two fractional powers

as only this guarantees that the zeroth order terms of the resulting power series in T

cancel each other.[3] We later saw that the additional introduction of a zeroth-order term via (16.35) likewise yields undesired powers in p and t. Continuing with using estimates that did not go as far and meant we sill had to integrate determinants, we realised that it is similarly important to

2. conserve the initial exponents of the charges n_I^i,

as these estimates led us to integrate only the minor of the charge matrix — i.e. with the overall exponent of the charges decreased by 1. This also resulted in an expression with altered powers in p and t.

While it seems that the first point above is important for the correct power in t and the second one for the correct power in p, there may be in fact more to it. First of all, changing the exponent of the charges n_I^i will of course result in an analogously different power in the p_I^i. At least when it comes to the t-dependency, both points may play a role. During our analytical computation of the basic building block in Section 14.2 and Appendix B, it was crucial that we did not just have a final Taylor series starting with a constant zeroth-order contribution. Instead, we faced the difference of two fractional powers with similar arguments, where the second one had an additional contribution $\sim T^2$ due to the shift — confer (B.54). With the lowest orders annulling each other via the difference, it was this additional T^2-term that caused the lowest order contribution to be $\sim t^2$. However, the second point above, about the power of the charges, can also affect the t-dependency. During the integration over the x_I^i, these integration variables are replaced by $\frac{p_I^i}{T}$ and, accordingly, modifying the exponent of the n_I^i results in altered powers in the integration variables x_I^i and therefore $\frac{p_I^i}{T}$, too.

So what we need is an estimate that only restructures the sum and the absolute values while keeping the difference in two terms that are $\sim n^{\frac{3r}{2}}$ — of which one also considers the shift. If we once more take a look at our estimate (16.35), we see that it looks quite promising if we neglect the $+2$,

$$\left|\sum_{\mathfrak{n}=1}^{N} \det \mathcal{N}_{\mathfrak{n}} + C\right|^{\frac{r}{2}} - \left|\sum_{\mathfrak{n}=1}^{N} \det \tilde{\mathcal{N}}_{\mathfrak{n}} + C\right|^{\frac{r}{2}} \overset{?}{\leq} \left[\left|n_1^1\right|^{\frac{r}{2}} - \left|n_1^1 + 1\right|^{\frac{r}{2}}\right] \left|\sum_{\mathfrak{n}=1}^{N} \Delta_1^1(\mathcal{N}_{\mathfrak{n}})\right|^{\frac{r}{2}}, \tag{16.64}$$

[3] Therefore, this also holds for estimates that result in an even number of terms with one half contributing with a plus sign and the other half with a minus sign.

and then estimate this expression by an integrable one:

$$(16.64) \leq \left[\left|n_1^1\right|^{\frac{r}{2}} - \left|n_1^1+1\right|^{\frac{r}{2}}\right] \sum_{\mathfrak{n}=1}^{N} \left|\Delta_1^1(\mathcal{N}_{\mathfrak{n}})\right|^{\frac{r}{2}}. \tag{16.65}$$

We already mentioned that we do indeed need this offset +2, but just to affirm our premise that an estimate of this kind would yield a desired result, we may still quickly check the final outcome. For this purpose, we can reuse our previous result of (16.46), where we just have to replace one $\sqrt{\pi}$ of the standard Gaussian-type integral over x_1^1 according to

$$\sqrt{\pi} \mapsto \int\limits_{-\infty}^{\infty} \mathrm{d}x_1^1 \, \frac{1}{T^s} \, \mathrm{e}^{-\left(x_1^1 - \frac{p_1^1 - \pi \mathrm{i} N_1^1}{T}\right)^2} \left(\left|x_1^1\right|^s - \left|x_1^1 + T\right|^s\right) \approx$$
$$\approx \frac{\Gamma\left(\frac{1}{2}\right)}{T^{2s}} \left(1 - \frac{s(1-s)}{4} \frac{T^2}{\left(p_1^1\right)^s}\right) \left(-s \frac{\left|p_1^1\right|^s}{p_1^1} T^2 + \frac{2(1-s)}{2} \frac{\left|p_1^1\right|^s}{\left(p_1^1\right)^2} T^4 + \mathcal{O}\left(T^6\right)\right), \tag{16.66}$$

coming from the Poisson resummation result of the square bracket in (16.65). Combining this with the remaining steps after (16.46), the lowest order contribution stemming from the incorrect estimate reads

$$\frac{\langle \hat{q}_1^1(r) \rangle_{\Psi_m}}{t} \overset{\times}{\leq} -\frac{r}{2} |Z|^{\frac{r}{2}} \sum_{IJ} \frac{\left|p_1^1 \Delta_1^1(p)\right|^{\frac{r}{2}}}{p_1^1} + \mathcal{O}(t). \tag{16.67}$$

Indeed, this expression features the desired dependency in both p and t: t^0 for the lowest order term as well as $\sim p^{\frac{3r}{2}-1}$, in accordance with the derivative-like action of the Poisson bracket. The composition is also a visible consequence of the estimates applied. We replaced the rational root of the absolute value of the sum of determinants by the difference of the rational root of the absolute value of the shifted and unshifted x_1^1, multiplied by the sum over all minors of the matrices of the x_I^i with respect to x_1^1. With all determinants that do not contain x_1^1 vanishing via the estimate, the remaining part of (16.67) resembles precisely this structure.

16.2.3 Comparison with the approach of Brunnemann and Thiemann

In this subsection, we aim at giving a comparison of the work of Brunnemann and Thiemann [65, 66] on calculating semiclassical expectation values of (products of) the class of operators $\hat{q}^{i_0}_{I_0}(r)$ and the new approaches that we presented in the work at hand. First of all, our analytical calculations of Section 14.2 only considered the monomial case $N = 1$ of one $\hat{q}^{i_0}_{I_0}(r)$. In Chapter 15, we then investigated general products $\prod_{k=1}^{N} \hat{q}^{j_k}_{J_k}(r)$ but were not able to access the cosmological singularity $p = 0$. Another difference is that Brunnemann–Thiemann obtain a diverging expression for the semiclassical limit $t \to 0$ — confer, e.g., the important choice of $r = \frac{1}{2}$ for their general case [65, (4.6)]$\sim t^{\left(\frac{3r}{2}-2\right)N}$ and [65, (4.7)]$\sim t^{\left(\frac{3r}{2}-1\right)N}$ for $p = 0$. In the present work, at least the rigorous computations of Section 14.2 featured the expected t-dependency.

We are therefore led to conclude that if we can access $p = 0$, then $t \to 0$ yields a diverging expression; and if we consider $t \to 0$, we can not as well investigate $p = 0$. Thinking about possible reasons for this, it seems that it is due to using estimates — at least for the first reasoning, with accessing $p = 0$ without estimates seems not possible so far. We already motivated that estimates may cause changes in the exponent of the charges and thereby of the integration variables and the final momenta, too. For a better understanding on how that comes about, we consider the t-dependency of the volume operator to the power of r:

$$\langle \hat{\mathrm{V}}^{r} \rangle_{\Psi_m} \sim {\ell_{\mathrm{P}}}^{3r} \sum \left| n^3 \right|^{\frac{r}{2}}. \tag{16.68}$$

If we now recap the steps from (16.9) to (16.15), we find that the integration of $\sum |n|^r$ against a Gaussian function results in an expression $\sim t^{-r}$. Therefore, we get with ${}^{\ell_{\mathrm{P}}}/_{a} = T = \sqrt{t}$ the desired t^0-dependency

$$\langle \hat{\mathrm{V}}^{r} \rangle_{\Psi_m} \sim {\ell_{\mathrm{P}}}^{3r} \sum \left| n^3 \right|^{\frac{r}{2}} \mapsto {\ell_{\mathrm{P}}}^{3r} t^{-\frac{3r}{2}} = a^{3r} \cdot t^0. \tag{16.69}$$

However, applying estimates so far means that there are at least some terms with a different exponent of the charges. This alters the above procedure of the "t-conversion" as the preceding factor ${\ell_{\mathrm{P}}}^{3r}$ remains as it is — it stems from looking at $\hat{\mathrm{V}}^{r}$ and sets the right dimension. Applying an estimate on the charges that changes their exponent then results in, e.g.,

$$\langle \hat{\mathrm{V}}^{r} \rangle_{\Psi_m} \sim {\ell_{\mathrm{P}}}^{3r} \sum \left| n^3 \right|^{\frac{r}{2}} \leq {\ell_{\mathrm{P}}}^{3r} \sum |n|^{2r} \mapsto {\ell_{\mathrm{P}}}^{3r} t^{-2r} = a^{3r} \cdot t^{-\frac{r}{2}}. \tag{16.70}$$

The unaffected prefactor ${\ell_{\mathrm{P}}}^{3r}$ can not fully compensate the new decreased exponent of t. We see this also happening in the $p = 0$ limit, where [65, (4.7)]$\sim t^{\frac{3r}{2}-2}$ (for $N = 1$ and including the additional division by t) and (16.19)$\sim t^{r-1}$ at the end of our similar but slightly different chain of estimates.

As a last remark on the Brunnemann–Thiemann approach, we discuss what seems to be one of the key quantities within their integration procedure. Between equations (5.3) and (5.7) in [66], Brunnemann–Thiemann introduce the variable A_I^i in a series of additional estimates and it is this quantity's constant contribution that ultimately constitutes the non-vanishing part in the limit $p \to 0$. With the integration procedure by means of KCHFs at hand, we can now investigate the importance of this new variable by explicitly computing the status of their calculations right before and after this step. We first adopt [66, (5.3)] to our notation:

$$[66,\ (5.3)] = \\ = \frac{{\ell_{\mathrm{P}}}^{3rN}(9M)^N|Z|^{\frac{rN}{2}}}{\sqrt{\pi}^{3M}t^N} \sum_{\{N_I^i\}\in\mathbb{Z}} \mathrm{e}^{-\sum_{Ii}\frac{\pi^2\left(N_I^i\right)^2}{t}} \int\limits_{-\infty}^{\infty} \mathrm{d}^{3M}x_I^i\ \mathrm{e}^{-\sum_{Ii}\left(x_I^i-\frac{p_I^i-\pi\mathrm{i}N_I^i}{T}\right)^2}\left(\sum_{Ii}\left(x_I^i\right)^2\right)^N, \tag{16.71}$$

where we directly included the norm of the state and completed the square within the Gaussian functions.[4] We can quite clearly integrate this expression with the methods introduced in Subsection 16.1.2, seeing that the above (16.71) is quite similar to (16.20) with $r = 2$ and $x_I^i \in \mathbb{R} \Rightarrow |x_I^i|^2 = (x_I^i)^2$. The prefactors ℓ_{P} and $|Z|$ are not affected by the estimates but $(9M)^{\frac{rN}{2}}$ indeed is — it originates from the sequence of estimates (16.9). If we set $r = 2$ therein, we can reproduce the estimate [66, (C.39)]. The calculatory steps then are the same as in Subsection 16.1.2 and we therefore just state the finale result

$$[66,\ (5.3)] \overset{t\to 0}{\leq} \left(27M^2\right)^N|Z|^{\frac{rN}{2}}(p_{\max})^{2N}t^{\left(\frac{3r}{2}-2\right)N} + \mathcal{O}\left(t^{\left(\frac{3r}{2}-2\right)N+1}\right). \tag{16.72}$$

Therein, to be able to find an overall upper bound, we again used $p_{\max} \coloneqq \max_{Ii}\{p_I^i\}$. In the same way, we get for the limit of the cosmological singularity

$$[66,\ (5.3)] \overset{p=0}{=} (9M)^N|Z|^{\frac{rN}{2}}t^{\left(\frac{3r}{2}-1\right)N}\sum_{\{n_{\mathfrak{k}}\}}\frac{c_{n_{\mathfrak{k}}}}{\sqrt{\pi}^{3M}}\prod_{Ii}\Gamma\left(n_{I,\mathfrak{k}}^i+\tfrac{1}{2}\right). \tag{16.73}$$

Hence, like before, we face incompletely cancelled normalisation constants $\sqrt{\pi}$. The over-

[4] We note that [66, (5.6) *et seq.*] lack the minus sign in the Gaussian functions in ${}^{\pi^2\left(N_I^i\right)^2}/_t$, which returns on page 30.

all factor $\sqrt{\pi}^{3M}$ first of all is reduced by all those $\Gamma(n^i_{I,\mathfrak{k}}+\frac{1}{2})$ with $n^i_{I,\mathfrak{k}}=0$. What is left is $\sqrt{\pi}^{\sharp(n^i_{I,\mathfrak{k}})}$, where we denote by $\sharp(n^i_{I,\mathfrak{k}})$ the number of $n_{\mathfrak{k}}\neq 0$ within the particular decomposition $n_{\mathfrak{k}}$. This corresponds to the number of non-standard-Gaussian type integrals resulting in $\Gamma(n^i_{I,\mathfrak{k}}+\frac{1}{2})$ instead of $\Gamma(\frac{1}{2})=\sqrt{\pi}$.

With this, we can now turn towards the integrals Brunnemann–Thiemann face directly after their introduction of A^i_I:

$$[66,\ (5.7)] = \frac{\ell_{\mathrm{P}}^{3rN}(9M)^N|Z|^{\frac{rN}{2}}}{\sqrt{\pi}^{3M}t^N}\sum_{\{N^i_I\}\in\mathbb{Z}} \mathrm{e}^{-\sum_{Ii}\frac{\pi^2\left(N^i_I\right)^2}{t}}\int\limits_{-\infty}^{\infty}\mathrm{d}^{3M}X^i_I\ \mathrm{e}^{-\sum_{Ii}\left(X^i_I\right)^2}\cdot$$
$$\cdot\left(\sum_{Ii}\left(A^i_I\left(X^i_I\right)^2-\frac{|p^i_I|A^i_I}{2T}+\frac{\pi^2\left(N^i_I\right)^2}{T^2}\right)\right)^N. \tag{16.74}$$

Before expanding the sum to the power of N, we may already now neglect all contributions with $N^i_I\neq 0$ — this is, of course, possible due to the preceding Gaussian in N^i_I. The much shorter expansion then reads

$$\left(\sum_{Ii}\left(A^i_I\left(X^i_I\right)^2-\frac{|p^i_I|A^i_I}{2T}\right)\right)^N = \sum_{\{n_{\mathfrak{k}}\}} d_{n_{\mathfrak{k}}}\prod_{Ii}\left(A^i_I\left(X^i_I\right)^2\right)^{n^i_{I,\mathfrak{k}}}\left(-\frac{|p^i_I|A^i_I}{2T}\right)^{m^i_{I,\mathfrak{k}}}. \tag{16.75}$$

Therein, we had to introduce a second kind of non-negative integer, $m^i_{I,\mathfrak{k}}$, as we did not have a sum of single terms to the power of N as before. The new pair $n^i_{I,\mathfrak{k}}, m^i_{I,\mathfrak{k}}$ of the decomposition $n_{\mathfrak{k}}$ of N into non-negative integers then follows $\sum_{Ii}\left(n^i_{I,\mathfrak{k}}+m^i_{I,\mathfrak{k}}\right)=N$ and

$$d_{n_{\mathfrak{k}}} := \frac{N!}{\prod_{Ii} n^i_{I,\mathfrak{k}}!\cdot m^i_{I,\mathfrak{k}}!} = \binom{N}{n^1_{1,\mathfrak{k}}, n^2_{2,\mathfrak{k}},\ldots,n^3_{M,\mathfrak{k}}, m^1_{1,\mathfrak{k}}, m^2_{2,\mathfrak{k}},\ldots,m^3_{M,\mathfrak{k}}}. \tag{16.76}$$

So what is the same as before is that we face the integration of Gaussian functions against the integration variable to the power of some even, non-negative integer. In contrast to before, we now do not have any offsets $\sim p^i_I$ or $\sim N^i_I$ in either parts of the integrand. Accordingly, the integrations can be solved via

$$\int\limits_{-\infty}^{\infty}\mathrm{d}X^i_I\ \mathrm{e}^{-\left(X^i_I\right)^2}\left(X^i_I\right)^{2n^i_{I,\mathfrak{k}}} = \Gamma\left(n^i_{I,\mathfrak{k}}+\tfrac{1}{2}\right) \tag{16.77}$$

and there is nothing further to do — especially no asymptotic expansions. Combining the formulae above, we have

$$[66,\ (5.7)] = \frac{t^{(\frac{3r}{2}-1)N}(9M)^N|Z|^{\frac{rN}{2}}}{\sqrt{\pi}^{3M}} \sum_{\{n_{\mathfrak{k}}\}} d_{n_{\mathfrak{k}}} \prod_{Ii} \big(A_I^i\big)^{n^i_{I,\mathfrak{k}}} \Gamma\big(n^i_{I,\mathfrak{k}} + \tfrac{1}{2}\big) \sqrt{\pi}^{m^i_{I,\mathfrak{k}}} \left(-\frac{|p_I^i|A_I^i|}{2T}\right)^{m^i_{I,\mathfrak{k}}}. \tag{16.78}$$

This also means that we can directly tackle the case of $p = 0$: Having $|p_I^i|^{m^i_{I,\mathfrak{k}}}$, we can say that the overall result will not vanish as for some of the decompositions $n_{\mathfrak{k}}$ of N it does indeed hold $m^i_{I,\mathfrak{k}} = 0\,\forall i, I$. The expression for $p = 0$ then reads

$$[66,\ (5.7)] \overset{p=0}{=} \frac{t^{\left(\frac{3r}{2}-1\right)N}(9M)^N|Z|^{\frac{rN}{2}}}{\sqrt{\pi}^{3M}} \sum_{\substack{\{n_{\mathfrak{k}}\}\text{ s.t.}\\ m^i_{I,\mathfrak{k}}=0\,\forall\, i,I}} d_{n_{\mathfrak{k}}} \prod_{Ii} \Gamma\big(n^i_{I,\mathfrak{k}} + \tfrac{1}{2}\big). \tag{16.79}$$

With these results, we can now deduce the effect of the introduction of A_I^i in [66]. Starting with the case of $p = 0$, we can say that both (16.73) and (16.79) are $\sim t^{\left(\frac{3r}{2}-1\right)N}$ — and this also holds for the final result of Brunnemann–Thiemann [66, (5.10) with $p = 0$]. For the general case, however, we found a t-dependence of $\sim t^{\left(\frac{3r}{2}-2\right)N}$ before their introduction of A_I^i, as (16.72) shows, while we obtained $\sim t^{\frac{3}{2}(r-1)N}$ for the expression right after the introduction of A_I^i, as (16.78) indicates when considering $\sum_{Ii} m^i_{I,\mathfrak{k}} = N$ to obtain the lowest order. Therefore, the introduction of A_I^i based on additional estimates does not play an important role concerning the initial singularity $p = 0$ and only causes a change in the combinatorical prefactors. When it comes to the introduction of A_I^i itself, it is not clear how this was done. Applying the binomial formula estimate within the sequence of steps from [66, (5.6] to [66, (5.7)] is in fact not possible due to $X_J^j \in \mathbb{C}$ and a similar question arises for the first line of that chain. Accordingly, the integration over X_I^i should in fact be complex. We point out that if one considers only the contributions $N_I^i = 0$ already from [66, (5.3)] onwards and does not introduce the absolute values, analogous computations can indeed be performed.

Chapter 17

Conclusion and outlook

17.1 Kummer's functions and coherent states on the circle

In the first part about Kummer's functions, we extended former results of [204–208] on coherent states on the circle in two different directions. We showed that we can compute semiclassical expectation values of fractional powers of the momentum operator by means of Kummer's confluent hypergeometric functions, which we have demonstrated in Section 11.3 and Subsection 12.2.1 for $L_2(\mathbb{R})$ and $L_2(S^1)$, respectively. For all operators considered in this part, the involved integrals were computed analytically without the need to perform any estimates during the calculations, as it has been done i.a. in [135] for fractional powers. Furthermore, since the asymptotic behaviour of Kummer's functions is well-known in this context, we can perform an expansion of these semiclassical expectation values in terms of the semiclassical parameter. It turns out that we automatically end up with the correct fractional power in the classical limit due to the fact that we do not need to estimate the integrals.

As a further result, we also discussed the computation of generic semiclassical matrix elements in the context of the Zak transformation and we were able to show that there exists a simple relation between semiclassical expectation values in $L_2(\mathbb{R})$ and $L_2(S^1)$ — as discussed in Subsection 12.2.2. Given an operator $\hat{O}_{\mathrm{QM}}$ that is well-defined on the set of coherent states, we can compute the associated matrix element $\langle T_{2\pi n}\Psi^{\hbar}_{q',p'} \,|\, \hat{O}_{\mathrm{QM}} \,|\, \Psi^{\hbar}_{q,p}\rangle$ in $L_2(\mathbb{R})$, where $T_{2\pi n}$ denotes a translation operator that translates by $2\pi n$ with $n \in$

$\mathbb{N}$. The matrix element for $L_2(S^1)$ can be expanded into a Fourier series whose Fourier coefficients c_n are then exactly given by $c_n = \langle T_{2\pi n}\Psi^{\hbar}_{q',p'} \,|\, \hat{O}_{\mathrm{QM}} \,|\, \Psi^{\hbar}_{q,p}\rangle$. This shows that the semiclassical matrix elements in $L_2(S^1)$ are completely determined by the corresponding "translated" matrix elements in $L_2(\mathbb{R})$. The variable in which the Fourier transform is evaluated is exactly the parameter δ used in [207, 208] that naturally enters the definition of the coherent states because it is the second argument of the Zak transform and for coherent states on the circle it can be understood as an additional fixed parameter in the interval 0 to 1. For a more detailed discussion on the physical properties of this parameter, see for instance [207]. Given this relation, semiclassical matrix elements like for instance in [135, 205, 206, 208, 208] can be computed in an alternative and possibly simpler manner. If we have an operator on $L_2(S^1)$ of which we want to compute semiclassical matrix elements, we just compute its Fourier coefficients, which in turn are simply matrix elements with respect to standard harmonic oscillator coherent states. Given these matrix elements, we can without any further computation directly write down the corresponding result for the matrix element in $L_2(S^1)$. We thereby avoid explicitly performing the Poisson resummation formula because that step is automatically taken care of by the procedure via the Zak transformation. This might likely reduce the actual effort of these semiclassical computations. Compared to the results of the expectation values in terms of Jacobi's theta functions and its derivatives as done in [205–207], we believe that the relation from Lemma 3 in equation (12.56) provides a more convenient alternative as far as the extraction of the classical limit is concerned.

Having restricted our considerations to coherent states on the circle, a natural question is whether the techniques introduced here can be generalised to more complicated situations. As already mentioned before, if we consider the Zak transform as a map from $L_2(\mathbb{R}^n)$ to $L_2(\mathbb{R}^{2n}/\mathbb{Z}^{2n})$, the relation of the matrix elements discussed in Subsection 12.2.2 carries over to the higher but finite dimensional case. As far as operators with fractional powers are concerned in a higher dimensional model, the operators can become more complicated functions of fractional powers than we considered here and thus it can happen that the integrals involved can no longer be solved by just using Kummer's functions. However, as we later discussed in Chapter 13 *et seq.*, similar techniques can be used for $\mathrm{U}(1)^3$ coherent states and a certain class of dynamical operators — generalisations of the operator considered at the end of Subsection 12.2.1 and also considered in [65, 66] —, which improve the final semiclassical expansion in certain aspects. In the context of loop quantum gravity, a generalisation from $\mathrm{U}(1)^3$ to $\mathrm{SU}(2)$ of this procedure would be beneficial to have at hand, in particular also because the semiclassical computations for SU(2) coherent states are much more involved in this case, so any simplification in this direction is welcome. Since the theta function can also be defined for SU(2) [235], we have a starting point for analysing in more detail whether a Zak transformation or a generalisation thereof can be used for SU(2) coherent states in a similar way.

17.2 Kummer's functions in loop quantum gravity

In the remainder of the work at hand, we extended the previously introduced method to analytically compute semiclassical expectation values based on Kummer's confluent hypergeometric functions to the case of $U(1)^3$ coherent states and the dynamical operators relevant in loop quantum gravity. We discussed this new procedure for computing semiclassical expectation values in addition to already existing ones in the loop quantum gravity literature. In particular, we investigated the question of singularity avoidance and compared our method to results by Brunnemann and Thiemann [65, 66]. The utilisation of Kummer's confluent hypergeometric functions allows to analytically evaluate integrals involving products of roots and Gaussians. Concerning the evaluation of these semiclassical expectation values, we differed between two main paths: The first one — covered in Chapter 14 and Chapter 15 — involves semiclassical computations that can be performed without estimates, whereas for the second path in Chapter 16 the calculations do rely on estimates. As a first scenario in the framework of loop quantum gravity, we considered graphs of cubic topology in Section 14.2, similar to the work of Sahlmann and Thiemann [63, 64], and aimed at computing semiclassical expectation values of the crucial dynamical operators $\hat{q}^{i_0}_{I_0}(r)$, products of which include for instance the analogue of the inverse scale factor in loop quantum gravity. Moreover, these operators are also involved in more complicated dynamical operators such as matter Hamiltonians or the Hamiltonian constraint of loop quantum gravity. We showed that for cubic graphs and linear power of $\hat{q}^{i_0}_{I_0}(r)$ our technique allows to compute the semiclassical expectation value of $\hat{q}^{i_0}_{I_0}(r)$ analytically without using estimates, as opposed to [65, 66], thereby extending results from the literature in the sense that the final outcomes still contain a stronger fingerprint of the initially involved fractional power r. The final expression for all semiclassical expectation values considered here can be written as a power series in the classicality parameter t and one expects to get the classical result in the limit where t is sent to zero. In the case of a graph of cubic topology and for non-vanishing classical triad labels of the complexifier coherent states, we were able to show that we obtain the correct classical limit in zeroth order of the classicality parameter without using estimates and, moreover, perform the continuum limit in which the regulator is removed as well. In the latter step, we were able to confirm in Section 14.4 that the regularisation constant of the volume operator for the $U(1)^3$ case needs to be $\frac{1}{48}$ in order to obtain the correct classical limit as was already pointed out in [64, 89, 90]. How this is related to the different result found in [236] — where the SU(2) case is considered using the graphical calculus — will be discussed in [234]. To analyse the singularity avoidance, we need to investigate the case in which the triad label of the coherent states vanishes, i.e. $p \to 0$. Then, the asymptotic expansion of Kummer's functions cannot be used in a similar manner as before; therefore, the computation of the semiclassical expectation value becomes more involved. As a consequence, we needed to introduce estimates in this specific case, which are however different to the ones used in [65, 66]. In accordance with their result, we also obtain a finite upper bound for the semiclassical value of $\hat{q}^{i_0}_{I_0}(r)$ for a graph of cubic topology and obtain singularity avoidance. However, the way how the fractional power enters into the final result differs and, as discussed in Section 14.3, therefore also for which values of the fractional power a finite expression in the $t \to 0$ limit exists. In our results, this happens if $\hat{q}^{i_0}_{I_0}(r)$ involves the volume operator linearly in the commutator, whereas for [65, 66] this is the case for a fractional power of the volume operator of $r = \frac{4}{3}$, showing, as rather expected, that such properties do highly depend on the kind of estimates used during the computations. The results discussed so far are restricted to linear powers of the operator $\hat{q}^{i_0}_{I_0}(r)$ and cubic graphs. The next, more involved case was considered in Chapter 15, where we recapitulated the procedure introduced by Sahlmann and Thiemann in [63, 64], which there was applied to cubic graphs. We extended this method to more general graphs and obtained, again up to some expected rescaling caused by the regularisation constant, the expected classical expression in the zeroth order of the classicality parameter. The case of $p = 0$, however, was not treatable with this procedure because it requires that the matrix built from the classical triad labels of the complexifier coherent states is invertible, which is no longer given in the limit $p \to 0$.

Concerning the second path covered in Chapter 16, we analysed whether our method based on Kummer's confluent hypergeometric functions can be used to improve the results for the upper bound regarding the singularity avoidance, that is the case $p = 0$. As discussed in the applications in Chapter 16, introducing estimates usually has the consequence that one estimates the original fractional powers by different powers in the classical label p, the classicality parameter t — or both. Compared to the estimates used in [65, 66], in some steps of our work we could keep fractional powers and did not need to estimate those by integer powers. Therefore, we aimed at trying to understand in more detail how the aforementioned modification of the order in t and p respectively arises when one uses estimates. As a first step, we carried out a computation that followed the path of [65, 66], where it was shown i.a. that there exists an upper bound for the semiclassical expectation value of the operator-analogue of the inverse scale factor even when approaching the initial singularity via $p = 0$. We modified the approach of [65, 66] in two ways: First, we did not need to get rid of the non-integer exponent of the charges as we could rely on the KCHF procedure. And secondly, the integration by means of KCHFs also allowed us to refrain from using additional estimates in order to evaluate the resulting integral. We discussed the case of one single $\hat{q}^{i_0}_{I_0}(r)$ and N-multiple ones separately in order to better demonstrate the differences and similarities of the two methods. Our result then features the same property when we want to consider $t \to 0$ additionally to $p = 0$ — or vice versa —, namely that the expression is not well defined if both limits are taken. We were able to find two aspects of estimates that cause this issue: One is changing the initial exponent of the charges via an estimate, causing ultimately a modified exponent of t as well. The other one is to apply estimates such that the initial difference due to the commutator is replaced by one single expression, whose integration then gives rise to one single KCHF and its power series. We saw during the analytical computation for graphs of cubic topology (cf. Section 14.2 and the last steps of Appendix B) that in the end, the zeroth order of the commutator's two KCHFs cancel each other — and this is of course not possible anymore when having only one function after using an estimate. Maybe one finds an estimate that changes the overall exponent in t, i.e. as a prefactor of the series, in such a way that this series' lowest order contribution turns out to carry the correct order in t, but the authors are not too positive about this possibility; and for such complicated operators this might also not be expected. Having these two reasons in mind, we continued to test new estimates that respect the "rules" of having a difference in KCHFs and not altering the U(1)-charges' exponents involved in the eigenvalue of the volume operator. However, for the analysed modified estimates in Section 16.2 there was always some issue occurring such that we ultimately had to break with one of the conditions — but our analysis gives a more detailed picture of where this exactly comes from in the application of the estimate. This can help to perform a future analysis on improved estimates in a more focused manner. For instance, one could use the ansatz for a new estimate that we stated at the end of Section 16.2 — where we showed that an intuitive, yet inapplicable estimate would yield the expected classical result — in order to reverse engineer a similar and indeed applicable estimate.

Another follow up question is whether there exists a link between the approaches via KCHFs and the Sahlmann and Thiemann one based on a Taylor expansion. Section 15.2 shows such a connection for the U(1) case, where one can associate the asymptotic expansion of the KCHF with the power series expansion of [64]. For higher-dimensional scenarios, however, this is not deducible in a similar straightforward manner as the KCHF way then means to successively perform the interwoven integrals. In contrast to this, the procedure Sahlmann and Thiemann used in [64] allows for tackling all integrations simultaneously after a disentanglement via a power series expansion.

A further and interesting generalisation of the methods presented in our work would be to extend the KCHF procedure for computing semiclassical expectation values and matrix elements to the case of SU(2) complexifier coherent states and understand how the techniques and results are related to the ones that one obtains via the semiclassical perturbation theory introduced in [60]. Besides that, there exists also work on matrix-valued KCHFs [237, 238, and references therein] that one may use in order to evaluate the integrals of the determinants. The authors looked into this but could not find a way to handle the calculations properly so far. However, the authors are also aware that this is still an active field of research and with investing more time, there might be ways to tackle it.

Summary

Chapter 18

Summary

We started this thesis with an introduction to loop quantum gravity in Part I *p. 3*, where we aimed at motivating the importance of the theory, its main ideas and concepts as well as specific frameworks that are relevant for what would follow — like coherent states.

Part II then covered the analysis of Gowdy models. We first introduced these models and motivated why they are of interest in Chapter 3 *p. 49*. The classical Gowdy model was then quantised in both reduced loop quantum gravity and algebraic quantum gravity. We chose for the first time a graph-preserving quantisation prescription for respecting the symmetries of the model also at the quantum level. Ultimately, we were interested in also finding first solutions to the Schrödinger-like equation of the Gowdy model quantised in algebraic quantum gravity. We started by constructing zero-volume eigenstates, which we used to outline the general procedure of how we can construct Gowdy states with specific, desired properties — namely by finding appropriate conditions for the coefficients within the linear combination of basis states such that the resulting state features that property. This allowed us to find also more complex states like ones that feature a vanishing action of the Euclidean part of the Hamiltonian. What is more, we could also discuss degeneracies of the action of the Lorentzian part. As possible next steps, we assume a perturbation theory approach can be of interest, where the symmetrised Euclidean part acts as a perturbation of the Lorentzian part [203]. Another direction would be to approach solutions to the evolved equations by means of numerical methods.
The more detailed conclusion on the Gowdy model investigations can be found in Chapter 8 *p. 115*.

Part III continued with semiclassical aspects of loop quantum gravity, while also laying the mathematical foundations of new procedures and illustratively applying them in standard quantum mechanics or for coherent states on a circle. We again started with an introduction and motivation, confer Chapter 9 *p. 121*. The main target of this part was to shed new light on the singularity avoidance in loop quantum gravity. For this, we introduced a new procedure that relies on Kummer's confluent hypergeometric functions and which allows us to compute semiclassical matrix elements and expectation values that can otherwise only be estimated. Carried over to standard quantum mechanics, the new procedure allows, e.g., to compute the semiclassical expectation value of fractional powers of the momentum operator. In loop quantum gravity, we can compute semiclassical matrix elements of a certain class of dynamical operators that can also be used to build the inverse scale factor. This allowed us to generalise and improve results from the literature concerning singularity avoidance. These new insights also allowed us to see Kummer's confluent hypergeometric functions themselves from a different angle — they are solutions to the heat equation — and find that the Zak transform can be used to map semiclassical matrix elements of coherent states on the circle to those of harmonic oscillator ones. As all these calculations were performed in Abelian scenarios, the consequential next step would be to analyse how we can extend the new procedures to SU(2).
The more detailed conclusion on the semiclassical considerations can be found in Chapter 17 *p. 231*.

Appendices

Appendix A

Ernst Eduard Kummer

Despite his achievements and his outstanding influence on the development of modern mathematics, Ernst Eduard Kummer is a name you hardly hear or read (at least the authors did not recognise him when they first encountered his confluent hypergeometric functions). We want to use this appendix to briefly motivate why this circumstance is very much unjustified and thereby pay tribute to this brilliant mathematician and influential teacher. We refer the interested reader to the more detailed biography by Hans–Joachim Girlich [240] as well as [241–244], which served as sources for this appendix.[1]

Figure A.1: Ernst Eduard Kummer [239]

One of the reasons why one barely encounters Ernst Eduard Kummer could be that he did not see too much value in writing books and instead only published scientific treatises. It is not even half a century ago that these were collectively published under the editorship of André Weil [226, 227]. However, this circumstance does not mean that he had no pedagogical abilities. Quite contrary, he enjoyed the reputation of being an

[1]We note that this appendix is supposed to be only a supplement to the thesis. It collects publicly available information on the life of Ernst Eduard Kummer, as the authors thought it may interest the reader as well. If so, we warmly recommend reading the references, too.

excellent teacher — with sometimes 250 students following his lectures — and being able to spark his students' interest on mathematical problems, while also offering personal and material support. When he was a school teacher in Legnica (then Liegnitz), two of his students were Leopold Kronecker and Ferdinand Joachimsthal — both of whom he could convince to pursue their mathematical talents. While Joachimsthal later took over Kummer's chair in Wrocław (then Breslau), he enjoyed a lifelong friendship with Leopold Kronecker, who later also became his student and whom he brought to Berlin when he was professor there. In Berlin, he took over the chair of Peter Gustav Lejeune Dirichlet, who moved to Göttingen. Together with Leopold Kronecker and Karl Weierstraß — whom he also got a professorship in Berlin —, he made Berlin the centre for mathematics. Notable doctoral students of his are Georg Cantor, Elwin Bruno Christoffel, Georg Frobenius, Wilhelm Killing, Leo August Pochhammer, Carl Runge, Arthur Schoenflies, Friedrich Schur and Hermann Amandus Schwarz [245], while he also supported Alfred Clebsch and Lazarus Fuchs — many names we already encountered in the main part of this thesis.

His mathematical achievements include work on hypergeometric functions — where we encountered his name — and laying the foundation for all future work on *Fermat's Last Theorem* by, i.a., introducing ideal numbers. For the latter, he was awarded the *Grand prix des sciences mathématiques* by the *Académie des sciences, Paris,* in 1857. The price was originally denoted for providing a solution to Fermat's Last Theorem, but with Kummer's work showing that all the current approaches have to fail and setting a new path for finding a solution, it was decided that this is an equally honourable achievement. With the help of these ideal numbers, he was able to show that Fermat's Last Theorem holds for all exponents that are multiples of regular primes. Further work of his was, i.a., on ray systems — a more geometrical topic — and ballistic problems.

In 1860, he was also elected as a member of the *Académie des sciences, Paris,* and in 1863 likewise for the *Royal Society, London*, while he was a member of the *Preußische Akademie der Wissenschaften, Berlin,* already from 1839 on. He retired in 1890 as he — and only he himself — noticed a diminishing capability of his memory. Three years later, he died in Berlin aged 83.

Appendix B

The 9 integrations

This appendix provides the integration of all the remaining integrals of Section 14.2. We directly start with

$$\frac{2}{t}\langle\hat{q}_1^1(r)\rangle_{\Psi_m} = \tag{B.1}$$

$$= \frac{2}{t}\frac{{\ell_{\mathrm{P}}}^{6r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9}{a^{6r}\|\Psi_m\|_-^2\, T^{3r}} \sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2} \int_{-\infty}^{\infty} \mathrm{d}^9 x_i \; \mathrm{e}^{-2\sum_i\left(x_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2} \Big(|\det X|^r - |\det \widetilde{X}|^r\Big),$$

where as before

$$X := \begin{pmatrix} x_1^1 & x_1^2 & x_1^3 \\ x_2^1 & x_2^2 & x_2^3 \\ x_3^1 & x_3^2 & x_3^3 \end{pmatrix} =: \begin{pmatrix} x_1 & x_2 & x_3 \\ x_4 & x_5 & x_6 \\ x_7 & x_8 & x_9 \end{pmatrix} \quad \text{and} \quad \widetilde{X} := \begin{pmatrix} x_1 + \frac{T}{2} & x_2 & x_3 \\ x_4 & x_5 & x_6 \\ x_7 & x_8 & x_9 \end{pmatrix}. \tag{B.2}$$

As mentioned during the introduction of Section 14.1, the integration variables x_i that we use correspond to the integration variables x_{Jj}^- of [64], while the remaining x_{Jj}^+ can be easily integrated over — they are of pure Gaussian type. In (B.2), we directly cancelled those contributions with one part of the norm of the coherent state, $\|\Psi\|_+^2$:

$$\|\Psi_m\|^2 = \underbrace{\left(\frac{2\pi\sqrt{\pi}}{T}\right)^9 \mathrm{e}^{2\sum_i\left(\frac{p_i^+}{T}\right)^2}}_{\|\Psi_m\|_+^2} \underbrace{\prod_i\Big(1+K_t^{(i)}\Big)\cdot\left(\frac{2\pi\sqrt{\pi}}{T}\right)^9 \mathrm{e}^{2\sum_i\left(\frac{p_i}{T}\right)^2}\prod_i\Big(1+K_t^{(i)}\Big)}_{\|\Psi_m\|_-^2} \tag{B.3}$$

$$= \|\Psi_m\|_+^2\,\|\Psi_m\|_-^2. \tag{B.4}$$

We absorbed both expansions $\prod_i \left(1 + K_t^{(i)}\right)$ into $\|\Psi_m\|_-^2$ to have more concise formulae at hand

Now, (B.2) is not integrable via our integration procedure by means of KCHFs and we therefore start with the substitution

$$x_1' := \det X, \tag{B.5}$$

$$x_{2,\ldots,9}' := x_{2,\ldots,9}, \tag{B.6}$$

with

$$\det\left(\frac{\mathrm{d}x'}{\mathrm{d}x}\right) = \det\begin{pmatrix} x_5x_9 - x_6x_8 & x_6x_7 - x_4x_9 & x_4x_8 - x_5x_7 & \ldots \\ 0 & 1 & 0 & \ldots \\ 0 & 0 & 1 & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = x_5x_9 - x_6x_8. \tag{B.7}$$

We therefore have to integrate

$$\frac{|x_1'|^r}{|x_5'x_9' - x_6'x_8'|}$$

against the Gaussian functions. At this point, we slightly deviate from the procedure started in Section 14.2 by also performing a second substitution right now:

$$x_5'' := x_5'x_9' - x_6'x_8', \tag{B.8}$$

$$x_{1,2,3,4,6,7,8,9}'' := x_{1,2,3,4,6,7,8,9}', \tag{B.9}$$

$$\det\left(\frac{\mathrm{d}x''}{\mathrm{d}x'}\right) = x_9'. \tag{B.10}$$

This leads us to integrating

$$\frac{|x_1''|^r}{|x_5''||x_9''|}$$

against the Gaussians and we got rid off the difference in the denominator. Note that this is the same substitution we announced in Section 14.2 after having performed the integration over x_1', and with $x_1' \mapsto x_1'' \equiv x_1'$ integrating over x_1'' is just equivalent to integrating over x_1' first. This integration over x_1'' now reads

$$\int\limits_{-\infty}^{\infty} \mathrm{d}x_1''|x_1''|^r \mathrm{e}^{-2\left(x_1''/x_5''+a\right)^2} = \sqrt{2}^{-1-r}\mathrm{e}^{-2a^2}|x_5''|^{1+r}\Gamma\left(\tfrac{1+r}{2}\right){}_1\mathrm{F}_1\left(\frac{1+r}{2}, \frac{1}{2}, 2a^2\right), \tag{B.11}$$

where we defined

$$a \coloneqq \frac{x_2''x_4''x_9'' + \frac{x_3''x_7''x_6''x_8''}{x_9''} - x_2''x_6''x_7'' - x_3''x_4''x_8''}{x_5''} + \frac{x_3''x_7''}{x_9''} - \frac{p_1 - \pi \mathrm{i} N_1}{T}, \tag{B.12}$$

which originates from considering $x_1' = x_1'(x_1, \ldots, x_9)$ and $x_1'' = x_1''(x_1', \ldots, x_9')$. The subsequent integration over x_5'' then has to also comprise all terms $\sim a = a(x_5'', \ldots)$:

$$\int_{-\infty}^{\infty} \mathrm{d}x_5''\ \mathrm{e}^{-2\left(x_5''/x_9''+b\right)^2} \mathrm{e}^{-2a^2} |x_5''|^r {}_1\mathrm{F}_1\left(\frac{1+r}{2}, \frac{1}{2}, 2a^2\right),$$

with

$$b \coloneqq \frac{x_6''x_8''}{x_9''} - \frac{p_5 - \pi \mathrm{i} N_5}{T}. \tag{B.13}$$

Just like during the treatment of Section 14.2, we now need to apply the asymptotic expansion for large arguments of the KCHF as integrals including a KCHF as well as an absolute value to the power of r are not feasible. With $a \sim \frac{1}{T}$, we can indeed perform the expansion, yielding

$$\mathrm{e}^{-2a^2} {}_1\mathrm{F}_1\left(\frac{1+r}{2}, \frac{1}{2}, 2a^2\right) \approx \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1+r}{2}\right)} \left(2a^2\right)^{\frac{r}{2}} \left(1 - \frac{r(1-r)}{4} \frac{a^{-2}}{2} + \mathcal{O}\left(\left(a^2\right)^{-2}\right)\right), \tag{B.14}$$

where — *as usual* — one of the expansion's series was damped by a preceding Gaussian function and can therefore be neglected. We now define $a =: \frac{c}{x_5''} + d$ to make the dependency on x_5'' palpable. Therein, c represents the numerator of that fraction of the definition of a, (B.12), that has x_5'' as its denominator and d collects the remaining contributions independent of x_5''. The integration over x_5'' up to now then is

$$\int_{-\infty}^{\infty} \mathrm{d}x_5''\ \mathrm{e}^{-2\left(x_5''/x_9''+b\right)^2} |x_5''|^r \left(2\left(\frac{c}{x_5''} + d\right)^2\right)^{\frac{r}{2}} \left[1 - \frac{r(1-r)}{8}\left(\frac{c}{x_5''} + d\right)^{-2}\right].$$

At this point, we may first consider the shifted contribution. We already introduced the integration over x_1 of this part in Section 14.2:

$$\int_{-\infty}^{\infty} \mathrm{d}x_1 |\det \widetilde{X}|^r\ \mathrm{e}^{-2\left(x_1 - \frac{p_1 - \pi \mathrm{i} N_1}{T}\right)^2} = \int_{-\infty}^{\infty} \mathrm{d}\tilde{x}_1 |\det X|^r\ \mathrm{e}^{-2\left(\tilde{x}_1 - \frac{p_1 + \frac{T^2}{2} - \pi \mathrm{i} N_1}{T}\right)^2}, \tag{B.15}$$

with $\tilde{x}_1 := x_1 + \frac{T}{2}$ and X as $X|_{x_1 \mapsto \tilde{x}_1}$ in abuse of notation. As mentioned earlier, this expression is just the one for the unshifted part with the only difference being $p_1 \mapsto p_1 + \frac{T^2}{2}$. However, be aware that within the (inverse) Gaussian functions including p_1 "outside" the integral, p_1 is not shifted.

We then perform the same steps as for the unshifted part and obtain

$$\int_{-\infty}^{\infty} \mathrm{d}x_1'' |x_1''|^r \mathrm{e}^{-2\left(x_1''/x_5'' + \tilde{a}\right)^2} = \sqrt{2}^{-1-r} \mathrm{e}^{-2\tilde{a}^2} |x_5''|^{1+r} \Gamma\left(\tfrac{1+r}{2}\right) {}_1\mathrm{F}_1\left(\frac{1+r}{2}, \frac{1}{2}, 2\tilde{a}^2\right), \tag{B.16}$$

where $\tilde{a} := a\big|_{p_1 \mapsto p_1 + \frac{T^2}{2}}$. The subsequent asymptotic expansion for large arguments of the KCHF therein yields

$$\int_{-\infty}^{\infty} \mathrm{d}x_1'' |x_1''|^r \mathrm{e}^{-2\left(x_1''/x_5'' + \tilde{a}\right)^2} \approx \frac{1}{\sqrt{2}} |x_5''|^{1+r} \Gamma\left(\tfrac{1}{2}\right) \left(\tilde{a}^2\right)^{\frac{r}{2}} \left(1 - \frac{r(1-r)}{4} \frac{\tilde{a}^{-2}}{2} + \mathcal{O}\left(\left(\tilde{a}^2\right)^{-2}\right)\right), \tag{B.17}$$

resulting in the integration over x_5'' of the contribution experiencing the shift as

$$\int_{-\infty}^{\infty} \mathrm{d}x_5''\ \mathrm{e}^{-2\left(\frac{x_5''}{x_9''} + b\right)^2} |x_5''|^r \left(\left(\frac{c}{x_5''} + d - \frac{T}{2}\right)^2\right)^{\frac{r}{2}} \left[1 - \frac{r(1-r)}{8} \left(\frac{c}{x_5''} + d - \frac{T}{2}\right)^{-2}\right].$$

From this form, we infer that the lowest order terms of the square brackets of the shifted and unshifted versions of the x_5''-integration do not just cancel each other for the shift being also present in the preceding factor to the power of $\frac{r}{2}$. Hence, we have to continue with performing the remaining integrations one after the other.

The next step was also already motivated in Section 14.2 and consists of performing a Taylor expansion of the square brackets. As we are ultimately interested in a power series in T, or in fact $t = T^2$, this is also just consequent. We then end up with the power series

$$\mathcal{S} := 1 - \frac{r(1-r)}{8} \frac{T^2}{{p_1}^2} + \mathcal{O}(T^3) \tag{B.18}$$

for indeed both square brackets — the one within the shifted as well as the unshifted part. Noticing that this expression does not include terms depending on x_5'' up to contributions $\sim T^2$, we managed to cast the square brackets into expressions that do not hinder the integration over x''_5 anymore. The reason why there is no N_1 within $\mathcal{S}$ leads to the last modification we have to undertake. The last part of the integrand that has to be modified now are the factors that are squared and taken to the power of $\frac{r}{2}$. Going back to our starting point, (B.2), we notice that there are still Gaussian prefactors in $\frac{N_i}{T}$. Therefore, we can discard all contributions $N_1 \neq 0$ — and will do so for all upcoming N_i, too —, as all those terms will be damped to zero for $t \to 0$. This means that now[1] $d \in \mathbb{R}$ and the squares to the power of $\frac{r}{2}$ become just the absolute value to the power of r: $\left((\ldots)^2\right)^{\frac{r}{2}} \mapsto |\ldots|^r$.[2]

With all this, we can now state the current status of our semiclassical expectation value:

$$
\begin{aligned}
&\frac{2}{t}\langle \hat{q}_1^1(r)\rangle_{\Psi_m} = \\
&= \frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9\Gamma\left(\frac{1}{2}\right)\mathcal{S}}{\|\Psi_m\|_-^2\sqrt{2}} \sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi \mathrm{i} N_i}{T}\right)^2} \int_{-\infty}^{\infty} \mathrm{d}^7 x''_{i\setminus 1,5}\ \mathrm{e}^{-2\sum_{i\setminus 1,5}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2} \frac{1}{|x''_9|}\cdot \\
&\quad\cdot \int_{-\infty}^{\infty} \mathrm{d}x''_5\ \mathrm{e}^{-2\left(\frac{x''_5}{x''_9}+b\right)^2}\left[|c+dx''_5|^r - \left|c+(d-\frac{T}{2})x''_5\right|^r\right] \qquad \text{(B.19)}\\
&= \frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9\Gamma\left(\frac{1}{2}\right)\mathcal{S}}{\|\Psi_m\|_-^2\sqrt{2}} \sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi \mathrm{i} N_i}{T}\right)^2} \int_{-\infty}^{\infty} \mathrm{d}^7 x''_{i\setminus 1,5}\ \mathrm{e}^{-2\sum_{i\setminus 1,5}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2} \frac{1}{|x''_9|}\cdot \\
&\quad\cdot \sqrt{2}^{-1-r}\Gamma\left(\tfrac{1+r}{2}\right)\left[\frac{1}{|d|}|dx''_9|^{1+r}\mathrm{e}^{-2\left(b-\frac{c}{dx''_9}\right)^2}{}_1\mathrm{F}_1\left(\frac{1+r}{2},\frac{1}{2},2\left(b-\frac{c}{dx''_9}\right)^2\right)-\right.\\
&\qquad\left.-\frac{1}{|d-\frac{T}{2}|}|(d-T)x''_9|^{1+r}\mathrm{e}^{-2\left(b-\frac{c}{(d-\frac{T}{2})x''_9}\right)^2}{}_1\mathrm{F}_1\left(\frac{1+r}{2},\frac{1}{2},2\left(b-\frac{c}{(d-\frac{T}{2})x''_9}\right)^2\right)\right]. \qquad \text{(B.20)}
\end{aligned}
$$

It now seems natural to continue with the integration over x''_9. The situation is very much like before: The integrand contains a KCHF that needs to transformed via the asymptotic expansion for large arguments — possible via $b \sim \frac{1}{T}$ —, where again only one of the sums will contribute and we directly apply a Taylor expansion afterwards, in order to have a

[1] For reasons of brevity and due to the limits of the alphabet, we continue using the letter d also for the quantity $d|_{N_1=0}$.

[2] Also for reasons of brevity, we do not modify the expression $\sum_{\{N_i\}\in\mathbb{Z}}\ \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}$ each time one of the N_i is set to zero.

power series in T. In the end, this leads to

$$\mathcal{S}' := 1 - \frac{r(1-r)}{8}\frac{T^2}{{p_5}^2} + \mathcal{O}(T^3), \tag{B.21}$$

setting already $N_5 = 0$. This is again justified by considering the Gaussian prefactor in $\frac{N_5}{T}$ that makes all contributions $N_5 \neq 0$ (exponentially) vanish. Just as before, it also transforms the square of the KCHF's argument to the power of $\frac{r}{2}$ into the absolute value of the KCHF's argument to the power of r. Hence, we are now facing

$$\begin{aligned}
\text{(B.20)} \approx \frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9\Gamma\left(\frac{1}{2}\right)^2\mathcal{S}\,\mathcal{S}'}{\|\Psi_m\|_-^2\sqrt{2}^2}\sum_{\{N_i\}\in\mathbb{Z}}\mathrm{e}^{2\sum\limits_i\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\int\limits_{-\infty}^{\infty}\mathrm{d}^6x''_{i\backslash 1,5,9}\;\mathrm{e}^{-2\sum\limits_{i\backslash 1,5,9}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\cdot\\
\cdot\int\limits_{-\infty}^{\infty}\mathrm{d}x''_9\;\mathrm{e}^{-2\left(x''_9-\frac{p_9-\pi\mathrm{i}N_9}{T}\right)^2}\left[\left|x''_9\left(x''_2x''_4-\frac{p_1p_5}{T^2}\right)+\frac{p_5}{T}x''_3x''_7+\frac{p_1}{T}x''_6x''_8-x''_2x''_6x''_7-x''_3x''_4x''_8\right|^r-\right.\\
\left.-\left|x''_9\left(x''_2x''_4-\frac{(p_1+\frac{T^2}{2})p_5}{T^2}\right)+\frac{p_5}{T}x''_3x''_7+\frac{p_1+\frac{T^2}{2}}{T}x''_6x''_8-x''_2x''_6x''_7-x''_3x''_4x''_8\right|^r\right]
\end{aligned} \tag{B.22}$$

$$\begin{aligned}
=\frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9\Gamma\left(\frac{1}{2}\right)^2\mathcal{S}\,\mathcal{S}'}{\|\Psi_m\|_-^2\sqrt{2}^2}\sum_{\{N_i\}\in\mathbb{Z}}\mathrm{e}^{2\sum\limits_i\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\int\limits_{-\infty}^{\infty}\mathrm{d}^6x''_{i\backslash 1,5,9}\;\mathrm{e}^{-2\sum\limits_{i\backslash 1,5,9}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\cdot\\
\cdot\sqrt{2}^{-1-r}\Gamma\left(\tfrac{1+r}{2}\right)\left[\left|x''_2x''_4-\frac{p_1p_5}{T^2}\right|^r\mathrm{e}^{-2\sigma^2}{}_1\mathrm{F}_1\left(\frac{1+r}{2},\frac{1}{2},2\sigma^2\right)-\right.\\
\left.-\left|x''_2x''_4-\frac{\left(p_1+\frac{T^2}{2}\right)}{T^2}\right|^r\mathrm{e}^{-2\tilde{\sigma}^2}{}_1\mathrm{F}_1\left(\frac{1+r}{2},\frac{1}{2},2\tilde{\sigma}^2\right)\right].
\end{aligned} \tag{B.23}$$

Therein, we abbreviated the peaks of the Gaussians as they are after a substitution making x''_9 the only argument of the absolute value according to

$$\sigma := \frac{-\frac{p_5}{T}x''_3x''_7-\frac{p_1}{T}x''_6x''_8+x''_2x''_6x''_7+x''_3x''_4x''_8}{x''_2x''_4-\frac{p_1p_5}{T^2}}-\frac{p_9-\pi\mathrm{i}N_9}{T}, \tag{B.24}$$

$$\tilde{\sigma} := \frac{-\frac{p_5}{T}x''_3x''_7-\frac{p_1+T^2/2}{T}x''_6x''_8+x''_2x''_6x''_7+x''_3x''_4x''_8}{x''_2x''_4-\frac{(p_1+T^2/2)p_5}{T^2}}-\frac{p_9-\pi\mathrm{i}N_9}{T}. \tag{B.25}$$

One feature of the procedure can already be noticed now: The numerator in (B.22) and (B.23) contains the numerical prefactor $\sqrt{2}^9$, stemming from the factor of 2 within the

Gaussians, which in turn entered our formulae via the substitution following (14.2). The successive integrations now build up a numerical prefactor $\sqrt{2}^n$ in the denominator that ultimately compensates the respective factor in the numerator.

From (B.23), we proceed as before and perform the asymptotic expansion of the two KCHFs — guaranteed as both σ and $\tilde{\sigma}$ are $\sim \frac{1}{T}$. The follow-up Taylor expansion (setting already $N_9 = 0$) then yields

$$\mathcal{S}'' := 1 - \frac{r(1-r)}{8}\frac{T^2}{{p_9}^2} + \mathcal{O}(T^3). \tag{B.26}$$

Therefore, we now have

$$\begin{aligned}
&(\text{B.23}) \approx \\
&\approx \frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9\Gamma\!\left(\frac{1}{2}\right)^3\mathcal{S}\mathcal{S}'\mathcal{S}''}{\|\Psi_m\|_-^2\sqrt{2}^3}\sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\int\limits_{-\infty}^{\infty}\mathrm{d}^5x''_{i\setminus 1,3,5,9}\ \mathrm{e}^{-2\sum_{i\setminus 1,3,5,9}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\cdot \\
&\quad\cdot\int\limits_{-\infty}^{\infty}\mathrm{d}x''_3\ \mathrm{e}^{-2\left(x''_3-\frac{p_3-\pi\mathrm{i}N_3}{T}\right)^2}\left[\left|x''_3\left(x''_4x''_8-\frac{p_5}{T}x''_7\right)+\tau\right|^r-\left|x''_3\left(x''_4x''_8-\frac{p_5}{T}x''_7\right)+\tilde{\tau}\right|^r\right] \\
&= \frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9\Gamma\!\left(\frac{1}{2}\right)^3\mathcal{S}\mathcal{S}'\mathcal{S}''}{\|\Psi_m\|_-^2\sqrt{2}^3}\sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\int\limits_{-\infty}^{\infty}\mathrm{d}^5x''_{i\setminus 1,3,5,9}\ \mathrm{e}^{-2\sum_{i\setminus 1,3,5,9}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\cdot \\
&\quad\cdot\frac{\Gamma\!\left(\frac{1+r}{2}\right)}{\sqrt{2}^{1+r}}\left|x''_4x''_8-\tfrac{p_5}{T}x''_7\right|^r\Bigg[\mathrm{e}^{-2\left(\frac{\tau}{x''_4x''_8-\frac{p_5}{T}x''_7}-\frac{p_3-\pi\mathrm{i}N_3}{T}\right)^2}{}_1\mathrm{F}_1\!\left(\frac{1+r}{2},\frac{1}{2},2\left(\frac{\tau}{x''_4x''_8-\frac{p_5}{T}x''_7}-\frac{p_3-\pi\mathrm{i}N_3}{T}\right)^2\right)- \\
&\qquad\qquad -\mathrm{e}^{-2\left(\frac{\tilde{\tau}}{x''_4x''_8-\frac{p_5}{T}x''_7}-\frac{p_3-\pi\mathrm{i}N_3}{T}\right)^2}{}_1\mathrm{F}_1\!\left(\frac{1+r}{2},\frac{1}{2},2\left(\frac{\tilde{\tau}}{x''_4x''_8-\frac{p_5}{T}x''_7}-\frac{p_3-\pi\mathrm{i}N_3}{T}\right)^2\right)\Bigg],
\end{aligned} \tag{B.27}$$

with

$$\tau := x''_2x''_6x''_7 - \frac{p_1}{T}x''_6x''_8 - \frac{p_9}{T}x''_2x''_4 + \frac{p_1p_5p_9}{T^3}, \tag{B.28}$$

$$\tilde{\tau} := x''_2x''_6x''_7 - \frac{p_1+\frac{T^2}{2}}{T}x''_6x''_8 - \frac{p_9}{T}x''_2x''_4 + \frac{\left(p_1+\frac{T^2}{2}\right)p_5p_9}{T^3}. \tag{B.29}$$

We see that we can again apply the asymptotic expansion for large arguments of the

KCHF on both KCHFs and with also performing the subsequent Taylor expansion we get

$$
\begin{aligned}
&(\text{B.27}) \approx \\
&\approx \frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9\Gamma\left(\frac{1}{2}\right)^4\mathcal{S}\mathcal{S}'\mathcal{S}''}{\|\Psi_m\|_-^2\sqrt{2}^4}\sum_{\{N_i\}\in\mathbb{Z}}\mathrm{e}^{2\sum\limits_i\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\int\limits_{-\infty}^{\infty}\mathrm{d}^4x''_{i=2,4,6,8}\;\mathrm{e}^{-2\sum\limits_{i=2,4,6,8}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\cdot \\
&\quad\cdot\int\limits_{-\infty}^{\infty}\mathrm{d}x''_7\;\mathrm{e}^{-2\left(x''_7-\frac{p_7-\pi\mathrm{i}N_7}{T}\right)^2}\left(1-\frac{r(1-r)}{8}\frac{x''^2_7\,T^4}{p_1{}^2p_9{}^2}\right)\left[\left|x''_7\left(x''_2x''_6-\frac{p_3p_5}{T^2}\right)+\omega\right|^r-\right. \\
&\qquad\left.-\left|x''_7\left(x''_2x''_6-\frac{p_3p_5}{T^2}\right)+\tilde{\omega}\right|^r\right]. \qquad (\text{B.30})
\end{aligned}
$$

As usual, only the $N_3=0$ contribution was considered and we abbreviated

$$
\omega := x''_8\left(\frac{p_3}{T}x''_4-\frac{p_1}{T}x''_6\right)-\frac{p_9}{T}x''_2x''_4+\frac{p_1p_5p_9}{T^3}, \qquad (\text{B.31})
$$

$$
\tilde{\omega} := x''_8\left(\frac{p_3}{T}x''_4-\frac{\left(p_1+\frac{T^2}{2}\right)}{T}x''_6\right)-\frac{p_9}{T}x''_2x''_4+\frac{\left(p_1+\frac{T^2}{2}\right)p_5p_9}{T^3}. \qquad (\text{B.32})
$$

This time, we do indeed face a different situation with the Taylor expansion's first non-constant contribution $1-\frac{r(1-r)}{8}\frac{(x''^2_7\,T^4)}{(p_1{}^2\,p_9{}^2)}$ being still dependent on the (next) integration variable x''_7. Even though it looks as if this term were contributing with T^4, it turns out to contribute with T^2 after the integration, just like the higher order contributions of all the Taylor expansions before. The important point now is that x''_7 is contained in the integrand with an integer power (and not within a KCHF, for example), allowing us to continue with the integration procedure via

$$
\begin{aligned}
\int\limits_{-\infty}^{\infty}\mathrm{d}x\;\mathrm{e}^{-\left(\frac{x}{c}+b\right)^2}|x|^r(x+d)^2 &= |c|^{1+r}\;\mathrm{e}^{-b^2}\Gamma\left(\tfrac{1+r}{2}\right)\left[d^2\,{}_1\mathrm{F}_1\left(\frac{1+r}{2},\frac{1}{2},b^2\right)+\right. \\
&\left.+\frac{1+r}{2}\,{}_1\mathrm{F}_1\left(\frac{3+r}{2},\frac{1}{2},b^2\right)-4\frac{1+r}{2}bcd\,{}_1\mathrm{F}_1\left(\frac{3+r}{2},\frac{3}{2},b^2\right)\right]. \qquad (\text{B.33})
\end{aligned}
$$

Also note that the Taylor expansion that caused this additional appearance of x''_7 did again not change the exponent of the integration variable, at least up to the first order in T. The asymptotic expansion for large arguments of the KCHF generates a series z^{-n} in the argument z of the KCHF. For both KCHFs in (B.27), the argument is $\sim(x''_7)^{-2}$ and therefore, the asymptotic expansion will contain a first order term $\sim(x''_7)^2$. Hence, the following Taylor expansion did not change the power of the integration variable x''_7.

Combining (B.33) & (B.30) and applying the asymptotic expansion on all six KCHFs, we obtain

$$
\begin{aligned}
&(\text{B.30}) \approx \\
&\approx \frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9 \Gamma\left(\frac{1}{2}\right)^5 \mathcal{S}\mathcal{S}'\mathcal{S}''}{\|\Psi_m\|_-^2\sqrt{2}^5} \sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi \mathrm{i} N_i}{T}\right)^2} \int_{-\infty}^{\infty} \mathrm{d}^3 x''_{i=2,4,6}\ \mathrm{e}^{-2\sum_{i=2,4,6}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2} \cdot \\
&\cdot \underbrace{\left(1-\frac{r(1-r)}{8}PT^2\right)}_{=:\mathcal{S}'''} \int_{-\infty}^{\infty} \mathrm{d}x''_8\ \mathrm{e}^{-2\left(x''_8-\frac{p_8-\pi\mathrm{i}N_8}{T}\right)^2}\left[\left|x''_8\left(\frac{p_3}{T}x''_4-\frac{p_1}{T}x''_6\right)+\chi\right|^r- \right.\\
&\qquad\left. -\left|x''_8\left(\frac{p_3}{T}x''_4-\frac{p_1+\frac{T^2}{2}}{T}x''_6\right)+\tilde{\chi}\right|^r\right],
\end{aligned}
\tag{B.34}
$$

where we defined

$$
P := \frac{{p_7}^2}{{p_1}^2\,{p_9}^2}+\frac{{p_3}^2}{\left(p_1p_9-p_3p_7\right)^2}, \tag{B.35}
$$

$$
\chi := x''_2\left(\frac{p_7}{T}x''_6-\frac{p_9}{T}x''_4\right)+\frac{p_1p_5p_9-p_3p_5p_7}{T^3} =: x''_2\left(\frac{p_7}{T}x''_6-\frac{p_9}{T}x''_4\right)+\frac{\mathcal{P}}{T^3}, \tag{B.36}
$$

$$
\tilde{\chi} := x''_2\left(\frac{p_7}{T}x''_6-\frac{p_9}{T}x''_4\right)+\frac{\mathcal{P}}{T^3}+\frac{p_5p_9}{2T}. \tag{B.37}
$$

Continuing, we get

$$
\begin{aligned}
&(\text{B.34}) \approx \\
&\approx \frac{2}{t}\frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9 \Gamma\left(\frac{1}{2}\right)^6 \mathcal{S}\mathcal{S}'\mathcal{S}''\mathcal{S}'''}{\|\Psi_m\|_-^2\sqrt{2}^6} \sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi \mathrm{i} N_i}{T}\right)^2} \int_{-\infty}^{\infty} \mathrm{d}^2 x''_{i=2,4}\ \mathrm{e}^{-2\sum_{i=2,4}\left(x''_i-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2} \cdot \\
&\cdot \int_{-\infty}^{\infty} \mathrm{d}x''_6\ \mathrm{e}^{-2\left(x''_6-\frac{p_6-\pi\mathrm{i}N_6}{T}\right)^2}\left(1-\frac{r(1-r)}{8}\frac{(p_3x''_4-p_1x''_6)^2T^4}{\mathcal{P}^2}\right)\left[\left|x''_6\left(\frac{p_7}{T}x''_2-\frac{p_1p_8}{T^2}\right)+\vartheta\right|^r- \right.\\
&\qquad\left. -\left|x''_6\left(\frac{p_7}{T}x''_2-\frac{\left(p_1+\frac{T^2}{2}\right)p_8}{T^2}\right)+\tilde{\vartheta}\right|^r\right],
\end{aligned}
\tag{B.38}
$$

with

$$\vartheta := x_4''\Big(\frac{p_3p_8}{T^2} - \frac{p_9}{T}x_2''\Big) + \frac{\mathcal{P}}{T^3}, \tag{B.39}$$

$$\tilde{\vartheta} := x_4''\Big(\frac{p_3p_8}{T^2} - \frac{p_9}{T}x_2''\Big) + \frac{\mathcal{P}}{T^3} + \frac{p_5p_9}{2T} \tag{B.40}$$

and we face again a prefactor that is not independent of the remaining integration variables. However, we can still perform the integration à la (B.33) even though there are now two integration variables involved. A rather long evaluation of all the usual steps then reveals

$$\begin{aligned}
&(\text{B.38}) \approx \\
&\approx \frac{2}{t}\frac{T^{3r}\Big(\frac{2\pi\sqrt{2}}{T}\Big)^9\Gamma\big(\frac{1}{2}\big)^7\mathcal{S}\mathcal{S}'\mathcal{S}''\mathcal{S}'''}{\|\Psi_m\|_-^2\sqrt{2}^7}\sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i\left(\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\int_{-\infty}^{\infty}\mathrm{d}^2x''_{i=2,4}\ \mathrm{e}^{-2\sum_{i=2,4}\left(x_i''-\frac{p_i-\pi\mathrm{i}N_i}{T}\right)^2}\cdot \\
&\cdot\underbrace{\left(1-\frac{r(1-r)}{8}\frac{{p_1}^2{p_6}^2\tilde{\mathcal{P}}^2+{p_1}^2{p_8}^2\mathcal{P}^2}{\tilde{\mathcal{P}}^2\mathcal{P}^2}T^2\right)}_{=:\mathcal{S}''''}\left[\left|x_4''\Big(\frac{p_3p_8}{T^2}-\frac{p_9}{T}x_2''\Big)+\frac{p_6p_7}{T^2}x_2''+\frac{\tilde{\mathcal{P}}}{T^3}\right|^r-\right. \\
&\qquad\left.-\left|x_4''\Big(\frac{p_3p_8}{T^2}-\frac{p_9}{T}x_2''\Big)+\frac{p_6p_7}{T^2}x_2''+\frac{\tilde{\mathcal{P}}}{T^3}+\frac{\Delta_1^1(p)}{2T}\right|^r\right],
\end{aligned} \tag{B.41}$$

where

$$\tilde{\mathcal{P}} := \mathcal{P} - p_1p_6p_8 = p_1p_5p_9 - p_3p_5p_7 - p_1p_6p_8 \tag{B.42}$$

continues to build up the determinant of the matrix of the p_i. Also, we defined

$$\Delta_1^1(p) := p_5p_9 - p_6p_8 \tag{B.43}$$

as the minor of that determinant with respect to $p_1 \equiv p_1^1$ where the shift happens:

$$\begin{pmatrix} p_1+\frac{T^2}{2} & p_2 & p_3 \\ p_4 & \boxed{\begin{matrix} p_5 & p_6 \\ p_8 & p_9 \end{matrix}} \\ p_7 & \end{pmatrix}. \tag{B.44}$$

Having resulted in an integration variable independent prefactor $\mathcal{S}''''$, we can integrate over x_4'' in the by now well-known manner:

$$(\text{B.41}) \approx \frac{2}{t} \frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9 \Gamma\left(\frac{1}{2}\right)^8 \mathcal{S}\mathcal{S}'\mathcal{S}''\mathcal{S}'''\mathcal{S}''''\mathcal{S}'''''}{\|\Psi_m\|_-^2 \sqrt{2}^8} \sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i \left(\frac{p_i - \pi \mathrm{i} N_i}{T}\right)^2} \int_{-\infty}^{\infty} \mathrm{d}x_2''\ \mathrm{e}^{-2\left(x_2'' - \frac{p_2 - \pi\mathrm{i}N_2}{T}\right)^2} \cdot$$
$$\cdot \left[\left| x_2'' \frac{p_6 p_7 - p_4 p_9}{T^2} + \frac{\hat{\mathcal{P}}}{T^3} \right|^r - \left| x_2'' \frac{p_6 p_7 - p_4 p_9}{T^2} + \frac{\hat{\mathcal{P}}}{T^3} + \frac{\Delta_1^1(p)}{2T} \right|^r \right], \tag{B.45}$$

with

$$\hat{\mathcal{P}} := \tilde{\mathcal{P}} + p_3 p_4 p_8 \tag{B.46}$$
$$\mathcal{S}'''''' := 1 - \frac{r(1-r)}{8} \frac{{p_3}^2 {p_8}^2}{\hat{\mathcal{P}}^2} T^2. \tag{B.47}$$

Before the final integration over x_2'', we can already see that the integrand of (B.45) looks very promising. First, with $\hat{\mathcal{P}}$ we have an expression that has nearly built up the determinant of the matrix of the p_i and the last missing terms are the ones including p_2. Knowing how the integration replaces the integration variable by the corresponding p_i divided by T, we see that these last contributions should be provided after the integration over x_2'': Within the absolute value to the power of r, x_2'' is multiplied by $p_6 p_7 - p_4 p_9$ which is just the minor of the matrix of the p_i with respect to p_2. Combined with $\hat{\mathcal{P}}$, this would sum up to $\det p$. Furthermore, the shifted contribution contains as an additional term compared to the unshifted part the minor of the matrix of the p_i with respect to p_1, $\Delta_1^1(p)$. This term is also of higher order in T, just as anticipated for the final result.

Now, the ultimate integration over x_2'' is of no unknown structure and we can analogously to the ones before perform the necessary steps, yielding

$$(\text{B.45}) \approx \frac{2}{t} \frac{T^{3r}\left(\frac{2\pi\sqrt{2}}{T}\right)^9 \Gamma\left(\frac{1}{2}\right)^9 \mathcal{S}\mathcal{S}'\mathcal{S}''\mathcal{S}'''\mathcal{S}''''\mathcal{S}'''''}{\|\Psi_m\|_-^2 \sqrt{2}^9} \sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{2\sum_i \left(\frac{p_i - \pi \mathrm{i} N_i}{T}\right)^2} \cdot$$
$$\cdot\, \mathcal{S}'''''' \left[\left| \frac{\det p}{T^3} \right|^r - \left| \frac{\det p}{T^3} + \frac{\Delta_1^1(p)}{2T} \right|^r \right], \tag{B.48}$$

with

$$\mathcal{S}''''''' := 1 - \frac{r(1-r)}{8} \frac{\left(p_6 p_7 - p_4 p_9\right)^2}{\left(\det p\right)^2} T^2 \tag{B.49}$$

and — finally — the determinant of the matrix of the p_i:

$$\det p := \hat{\mathcal{P}} + p_2 p_6 p_7 - p_2 p_4 p_9. \tag{B.50}$$

As a last step, we include the remaining part of the norm of the coherent state,

$$\|\Psi_m\|_-^2 = \prod_i \Big(1 + K_t^{(i)}\Big) \left(\frac{2\pi\sqrt{\pi}}{T}\right)^9 \mathrm{e}^{2\sum_i \left(\frac{p_i}{T}\right)^2} \prod_i \Big(1 + K_t^{(i)}\Big), \tag{B.51}$$

multiply the expansion-series-like prefactors and combine the contributions of the shifted and unshifted parts. Recap that in (B.51), $K_t^{(i)} = \mathcal{O}(t^\infty)$, i.e. $\lim_{t\to 0} K_t^{(i)}/t^n = 0\ \forall n \in \mathbb{N}$ [66]. The reason for this is again that for

$$\prod_i \Big(1 + K_t^{(i)}\Big) := \sum_{\{N_i\}\in\mathbb{Z}} \mathrm{e}^{-2\sum_i \left(\frac{\pi^2 {N_i}^2}{T^2} + \frac{2\pi \mathrm{i} p_i N_i}{T^2}\right)}, \tag{B.52}$$

only the solution $\{N_i\} = 0$ will contribute, while all other are exponentially damped. The inverse Gaussian factors $\mathrm{e}^{2\sum_i \left(\frac{p_i}{T}\right)^2}$ within the norm of the coherent state compensate $\mathrm{e}^{2\sum_i \left(\frac{p_i - \pi \mathrm{i} N_i}{T}\right)^2}$ of (B.45), having in mind that $\{N_i\} = 0$. As an intermediate result, we therefore now have

$$\frac{2}{t}\langle \hat{q}_1^1(r)\rangle_{\Psi_m} \approx \frac{2}{t} \frac{\Gamma\left(\frac{1}{2}\right)^9 T^{3r} \mathcal{S}\mathcal{S}'\mathcal{S}''\mathcal{S}'''\mathcal{S}''''\mathcal{S}'''''\mathcal{S}''''''}{\sqrt{\pi}^9 \prod_i \Big(1 + K_t^{(i)}\Big) \prod_i \Big(1 + K_t^{(i)}\Big)} \left[\left|\frac{\det p}{T^3}\right|^r - \left|\frac{\det p}{T^3} + \frac{\Delta_1^1(p)}{2T}\right|^r\right]. \tag{B.53}$$

First, we can say that the normalisation prefactors cancel as $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$. The rest of the expression is just as expected: We face a difference in the absolute value to the power of r of a unshifted and shifted contribution, multiplied by power-series-like prefactors $(1 - \frac{r(1-r)}{8} f(\{p_i\})\, T^2)$. We can now use the remaining T^{3r} to reformulate the difference of the unshifted an shifted part as

$$\begin{aligned} T^{3r}\left[\left|\frac{\det p}{T^3}\right|^r - \left|\frac{\det p}{T^3} + \frac{\Delta_1^1(p)}{2T}\right|^r\right] &= |\det p|^r - \left|\det p + \Delta_1^1(p)\frac{T^2}{2}\right|^r \\ &\approx -r\frac{|\det p|^r \Delta_1^1(p)}{\det p}\frac{T^2}{2} - \frac{r(r-1)}{8}\frac{|\det p|^r (\Delta_1^1(p))^2}{|\det p|^2} T^4 + \mathcal{O}\big(T^6\big). \end{aligned} \tag{B.54}$$

For the very last step, we insert this into (B.53) and multiply all $\mathcal{S}^{(\prime\ldots\prime)}$ to obtain

$$\frac{2}{t}\langle\hat{q}_1^1(r)\rangle_{\Psi_m} \approx -\frac{2}{t}r\frac{|\det p|^r\Delta_1^1(p)}{\det p}\frac{T^2}{2} + \frac{2}{t}\mathcal{F}T^4 + \frac{2}{t}\mathcal{O}(T^5). \tag{B.55}$$

The zeroth order contribution

$$r\frac{|\det p|^r\Delta_1^1(p)}{\det p}$$

then perfectly resembles the result of the Poisson bracket of the corresponding classical expressions. During the last step, this contribution was the result of the term $\sim T^2$ of (B.54) multiplied by all 1s from the $\mathcal{S}^{(\prime\ldots\prime)}$. Due to all these factors being series à la $1 - \ldots T^2 + \mathcal{O}(T^3)$ and (B.54) being of the form $\ldots T^2 + \ldots T^4 + \mathcal{O}(T^6)$, we were able to also state the next higher order term $\sim T^4$: All final terms $\sim T^4$ are either the term $\sim T^4$ of (B.54) multiplied by all the 1s of the $\mathcal{S}^{(\prime\ldots\prime)}$, or the term $\sim T^2$ of (B.54) multiplied by the sum of all terms $\sim T^2$ of the $\mathcal{S}^{(\prime\ldots\prime)}$. Note that had we included also terms $\sim T^3$ within the $\mathcal{S}^{(\prime\ldots\prime)}$, those would be multiplied at least with the term $\sim T^2$ of (B.54), therefore resulting in an overall term $\sim T^5$. We then collected all those terms $\sim T^4$ in

$$\begin{aligned}\mathcal{F} :=& -\frac{r(r-1)}{8}\frac{|\det p|^r\left(\Delta_1^1(p)\right)^2}{|\det p|^2} - \frac{r^2(r-1)}{16}\frac{|\det p|^r\Delta_1^1(p)}{\det p}\left[\frac{1}{{p_1}^2} + \frac{1}{{p_5}^2} + \frac{1}{{p_9}^2} + P + \right.\\ &\left. + \frac{{p_1}^2{p_6}^2\tilde{\mathcal{P}}^2 + {p_1}^2{p_8}^2\mathcal{P}^2}{\tilde{\mathcal{P}}^2\mathcal{P}^2} + \frac{{p_3}^2{p_8}^2}{\hat{\mathcal{P}}^2} + \frac{(p_6p_7 - p_4p_9)^2}{(\det p)^2}\right].\end{aligned} \tag{B.56}$$

Checking the overall powers in the p_i for all terms of (B.56), we need to have in mind that $P \overset{(B.35)}{=} \frac{{p_7}^2}{{p_1}^2{p_9}^2} + \frac{{p_3}^2}{(p_1p_9 - p_3p_7)^2}$, i.e. $P \sim p^{-2}$, while all of $\mathcal{P}, \tilde{\mathcal{P}}, \hat{\mathcal{P}}$ are $\sim p^3$. Therefore, the first term does indeed have a different overall power in the p_i than the remaining ones: p^{3r-2} vs. p^{3r-3}. This feature of the next-to-leading order term containing two contributions with different powers in the fluxes/momenta can also be seen in the quantum mechanical case, confer (11.35) and (11.38). However, in (4.45) of [64], this behaviour is not observed as all terms there are $\sim p^{3\frac{r}{2}-3}$ for $N = 1$. We assume the reason for this is the power counting performed in (4.39) of [64]: There, the point is made that one could neglect terms $\sim sT$ compared to terms $\sim s^2$, where $s = t^{\frac{1}{2}-\alpha}$. α was defined via $p \mapsto q := pt^{-\alpha}$ in order to have a quantity "of order unity". This s is always paired with q^{-1} as there should be no trace of α in the final result. Therefore, $sT = t^{1-\alpha}$ is of higher order in t than $s^2 = t^{1-2\alpha}$, as $\alpha > 0$. However, all terms $\sim sT$ are combined with q^{-1}, causing them to be $\sim t$ — just like all terms $\sim s^2$, which are paired with q^{-2}. Now, this term $\sim sT$ that was not considered anymore contains one less inverse q compared to the term

s^2, making it of higher order in p than the one included in the final result. With the final result of [64] containing terms $\sim p^{3\frac{r}{2}-3}$ in the contribution $\sim t$, this is in accordance with the observation that (B.56) also contains a part $\sim p^{3r-2}$ — note that we used r, where [64] used $\frac{r}{2}$. Accordingly, the correction terms [64] considers should be the same as the ones of the second part of (B.56) above. This can even be motivated by both the quantum mechanical and the U(1) case, confer the discussion following (15.17), as they should be the derivative of the fluctuations of the expectation value of the volume operator. However, finding a stringent link between the two procedures was not possible so far. For the U(1) case, Section 15.2 offers a connection but for the higher dimensional case, the procedures deviate too much. For the correction term $\sim sT$ that was neglected in [64, cf. eq. (4.39)], it is in turn quite straightforward to check that it corresponds to the first part of (B.56).

Appendix C

Estimates

This is a list of the fundamental estimates that we use during our considerations on semiclassical expectation values of the class of operators $\hat{q}^{i_0}_{I_0}(r)$.

- Brunnemann and Thiemann [66] used the estimate

$$|a|^r - |b|^r \leq ||a| - |b|| \quad \text{(where } a, b \in \mathbb{Z} \text{ and } r \in \mathbb{Q}_{[0,1]}) \tag{C.1}$$

  to get rid of the roots.

- With the help of

$$|a|^r - |b|^r \leq |a - b|^r \quad \text{(where } a, b, r \in \mathbb{R} \text{ and } 0 \leq r \leq 1), \tag{C.2}$$

  we replace the difference in roots by a single root. We can then perform further modifications of the term corresponding to $(a-b)$, allowing us in the end to integrate the expression against Gaussians by means of KCHFs.

- For the root of a sum, the — to some extend — equivalent but reverse estimate reads

$$|a + b|^r \leq |a|^r + |b|^r \quad \text{(where } a, b, r \in \mathbb{R} \text{ and } 0 \leq r \leq 1), \tag{C.3}$$

  which we will also need.

- We will use

$$|a+C|^r - |(a-1)+C|^r \leq |a|^r - |a-1|^r + 2 \quad \text{(where } a, C, r \in \mathbb{R} \text{ and } 0 \leq r \leq 1) \tag{C.4}$$

during our search for a "good" estimate for the case of $\mathrm{U}(1)^3$.

Using (C.2), we can straightforwardly proof this estimate:

$$\begin{aligned} |a+C|^r - |a+\delta+C|^r + |a+\delta|^r - |a|^r &\leq |a+C-(a+\delta+C)|^r + |a+\delta-a|^r \\ &= 2|\delta|^r. \end{aligned} \tag{C.5}$$

The important part of the estimates (C.2), (C.3) and (C.4) is that they still contain $|\ldots|^r$, i.e. the initial exponent r, while (C.1) does not.

Appendix D

The semiclassical continuum limit for graphs of cubic topology

This appendix covers the derivation of the result we already presented in Section 14.4 concerning the semiclassical continuum limit for graphs of cubic topology. We stated that in this scenario, taking both limits $t \to 0$ and $\epsilon \to 0$ — i.e. having the classicality parameter and the lattice regularisation parameter vanish — reproduces the classical Poisson bracket:

$$\lim_{t\to 0} \frac{2\langle \hat{q}^{i_0}_{I_0}(r)\rangle_{\Psi_m}}{t} = -r\frac{\left|\det p^-\right|^r \Delta^{i_0}_{I_0}(p^-)}{\det p^-} = 2\mathrm{i}h^{i_0}_{I_0}\Big\{\big(h^{i_0}_{I_0}\big)^{-1}, V^{2r}(R_{\Box_\epsilon})\Big\} \tag{D.1}$$

$$\lim_{\epsilon\to 0}\Big(2\mathrm{i}h^{i_0}_{I_0}\Big\{\big(h^{i_0}_{I_0}\big)^{-1}, V^{2r}(R_{\Box_\epsilon})\Big\}\Big) = \frac{1}{a^{6r}}\left\{\int_{e_{I_0}} A^{i_0}, V^{2r}(R_x)\right\}. \tag{D.2}$$

Therein, i entered the formulae as we work with $\mathrm{U}(1)^3$ instead of $\mathrm{SU}(2)$, the quantisation is performed by additionally dividing by $\frac{1}{\mathrm{i}\hbar}$ and $\frac{1}{a^{6r}}$ is considered in order to work with a dimensionless volume — confer (10.5). We already mentioned in Section 14.4 that we have to include an extra factor of 2 for getting the correct semiclassical limit of the Thiemann identity (see [234]).

We start by showing that the classical identity

$$h^{i_0}_{I_0}\Big\{\big(h^{i_0}_{I_0}\big)^{-1}, V^{2r}(R_{\Box_\epsilon})\Big\} = -\mathrm{i}\frac{\kappa}{2a^2}r\left|\det p^-\right|^r\frac{\Delta^{i_0}_{I_0}(p^-)}{\det p^-} \equiv -\mathrm{i}\frac{\kappa}{2a^2}r\left|\det p^-\right|^r\big((p^-)^{-1}\big)_{I_0 i_0} \tag{D.3}$$

holds for cubic graphs in the $U(1)^3$ setup. For the Poisson bracket, we have

$$h_{I_0}^{i_0}\Big\{\big(h_{I_0}^{i_0}\big)^{-1}, V^{2r}(R_{\square_\epsilon})\Big\} = \kappa h_{I_0}^{i_0}\int \mathrm{d}^3 z\left(\frac{\delta(h_{I_0}^{i_0})^{-1}}{\delta A_b^k(z)}\right)\left(\frac{\delta V^{2r}(p^-)}{\delta E_k^b(z)}\right), \tag{D.4}$$

where we can rephrase the two factors of the integrand as

$$h_{I_0}^{i_0}\left(\frac{\delta(h_{I_0}^{i_0})^{-1}}{\delta A_b^k(z)}\right) = -\mathrm{i}\int_0^1 \mathrm{d}t\, \dot{e}_{I_0}^a(t)\delta^{k i_0}\delta_b^a\delta(t,z) \tag{D.5}$$

and

$$\left(\frac{\delta V^{2r}(p^-)}{\delta E_k^b(z)}\right) = r\big|\det p^-\big|^{r-1}\,\mathrm{sgn}(p^-)\left(\frac{\delta \det p^-}{\delta E_k^b(z)}\right), \tag{D.6}$$

respectively. For determining the functional derivative of the last identity, we need to reintroduce the $p_{I_0\sigma_0 i_0}$ as in [64]. Recap that the subscripts denote the edges $I_0 = 1,2,3$, the U(1)-copy $i_0 = 1,2,3$ as well as the sign $\sigma_0 = \pm$ that tells whether the edge is in- or outgoing. With a follow-up insertion of the fluxes

$$E_{j\sigma}^J := \int_{S_{e_J^\sigma}} E_j^a n_a^{S_{e_J^\sigma}}, \tag{D.7}$$

we have

$$p_{I_0 i_0}^- = \frac{1}{2}(p_{I_0+i_0} - p_{I_0-i_0}) = \frac{1}{2a^2}\big(E_{i_0+}^{I_0} - E_{i_0-}^{I_0}\big), \tag{D.8}$$

$$p_{I_0 i_0}^+ = \frac{1}{2}(p_{I_0+i_0} + p_{I_0-i_0}) = \frac{1}{2a^2}\big(E_{i_0+}^{I_0} + E_{i_0-}^{I_0}\big). \tag{D.9}$$

In (D.7), $S_{e_J^\sigma}$ denotes the surface that is dual to the edge e_J^σ and $n_a^{S_{e_J^\sigma}}$ then is the respective conormal of that surface. For the latter, we use the shorthand notation $n_a^{J\sigma} := n_a^{S_{e_J^\sigma}}$. This yields

$$\left(\frac{\delta \det p^-}{\delta E_k^b(z)}\right) = \frac{\det p^-}{2a^2}\big((p^-)^{-1}\big)_{Jj}\left(\int_{S_{e_J^+}} \mathrm{d}^2 u\, n_a^{J+}\delta_j^k\delta_b^a\delta(x(u),z) - \int_{S_{e_J^-}} \mathrm{d}^2 u\, n_a^{J-}\delta_j^k\delta_b^a\delta(x(u),z)\right). \tag{D.10}$$

Combining (D.5) and (D.10) with (D.4), we reproduce (D.3) via

$$\begin{aligned} h^{i_0}_{I_0}\Big\{\big(h^{i_0}_{I_0}\big)^{-1}, V^{2r}(R_{\square_\epsilon})\Big\} &= -\frac{\mathrm{i}\kappa}{2a^2} r \big|\det p^-\big|^{r-1}\big|\det p^-\big|\big((p^-)^{-1}\big)_{I_0 i_0} \\ &= -\frac{\mathrm{i}\kappa}{2a^2} r \big|\det p^-\big|^{r} \frac{\Delta^{i_0}_{I_0}(p^-)}{\det p^-}. \end{aligned} \tag{D.11}$$

Note that we also used $\Delta^{i_0}_{I_0}(p^-) = \frac{1}{2}\epsilon^{i_0 k\ell}\epsilon_{I_0 KL} p^-_{Kk} p^-_{L\ell}$ in the last step.

Having in mind

$$p_{I_0+i_0} = p^+_{I_0 i_0} + p^-_{I_0 i_0} \quad \wedge \quad p_{I_0-i_0} = p^+_{I_0 i_0} - p^-_{I_0 i_0} \qquad \Longleftrightarrow \qquad p_{I_0\sigma_0 i_0} = p^+_{I_0 i_0} + \mathrm{sgn}(\sigma_0) p^-_{I_0 i_0},$$

we can reformulate $((p^-)^{-1})_{I_0 i_0} =: (p^-_{I_0 i_0})^{-1}$ as

$$\mathrm{sgn}(\sigma_0)(p^-_{I_0 i_0})^{-1} = (\mathbb{1} - p^{-1}_{I_0\sigma_0 i_0}(p^+_{I_0 i_0}))^{-1} p^{-1}_{I_0\sigma_0 i_0}. \tag{D.12}$$

Therein, we used the superscript $^{-1}$ to mark the inverse of the corresponding matrix and the subscripts then specify the matrix element one currently considers. For $p^{-1}_{I_0\sigma_0 i_0}$, we then get

$$p^{-1}_{I_0\sigma_0 i_0} = \frac{1}{2}\epsilon^{i_0 mn}\epsilon^{I_0 MN}\frac{p_{M\sigma_0 m} p_{N\sigma_0 n}}{\det p_{\sigma_0}} = \frac{a^2}{2}\epsilon^{i_0 mn}\epsilon^{I_0 MN}\frac{E^M_{m\sigma_0} E^N_{n\sigma_0}}{\det E_{\sigma_0}},$$

with the already used notational convention $\det E_{\sigma_0} \equiv \det\big(E^J_{j\sigma_0}\big)$. Being interested in expanding both the fluxes and their just mentioned determinant in powers of the lattice regularisation parameter, we introduce the embedding

$$X^a_v\colon \Big[-\frac{\epsilon}{2}, \frac{\epsilon}{2}\Big] \to \sigma, \quad (t^1, t^2, t^3) \mapsto X^a_v(t_1, t_2, t_3), \quad X^a_v(0,0,0) = v.$$

We can then perform the two expansions as

$$E^J_{j\sigma} = \epsilon^2 E^a_j(v) n^{J\sigma}_a(v) + \mathcal{O}\big(\epsilon^3\big) \quad \text{and} \tag{D.13}$$

$$\begin{aligned} \det E_\sigma \equiv \det\big(E^J_{j\sigma}\big) &= \det\big(\epsilon^2 E^a_j(v) n^{J\sigma}_a(v) + \mathcal{O}\big(\epsilon^3\big)\big) = \epsilon^6 \det\big(E^a_j(v)\big)\det\big(n^{J\sigma}_a(v)\big) + \mathcal{O}\big(\epsilon^7\big) \\ &= \epsilon^6 \det E(v)\cdot \det n^\sigma(v) + \mathcal{O}\big(\epsilon^7\big). \end{aligned} \tag{D.14}$$

We now have $\det E(v) \equiv \det\big(E^a_j(v)\big)$, where the E^a_j are linked to the $E^J_{j\sigma_0}$ by means of (D.7), and $\det n^\sigma(v) \equiv \det\big(n^{J\sigma}_j(v)\big)$. Having in mind that $n^{J+}_a(v) = -n^{J-}_a(v)$ and with

$p^+_{I_0 i_0}$ formulated as in (D.9), we conclude that the leading order vanishes. With that, the contribution $\sim p^{-1}_{I_0\sigma_0 i_0} p^+_{I_0 i_0}$ in (D.12) is of higher order in the lattice regularisation parameter ϵ compared to the part with the unit matrix $\mathbb{1}$ and can therefore be neglected when considering $\epsilon \to 0$. We therefore have for (D.12)

$$\operatorname{sgn}(\sigma_0)(p^-_{I_0 i_0})^{-1} = \operatorname{sgn}(\sigma_0)\frac{a^2}{2}\epsilon^{i_0 mn}\epsilon^{I_0 MN}\frac{E^a_m n^{M\sigma_0}_a E^b_n n^{N\sigma_0}_b}{\det E(v)|\det n^\sigma(v)|}\left(\frac{1+\mathcal{O}(\epsilon)}{\epsilon^2+\mathcal{O}(\epsilon^3)}\right), \tag{D.15}$$

where the sgn accounts for the absolute value we introduced in the denominator.

For the expansion of (D.3), all this yields

$$h^{i_0}_{I_0}\Big\{\big(h^{i_0}_{I_0}\big)^{-1}, V^{2r}(R_{\square_\epsilon})\Big\} = -\mathrm{i}\frac{\kappa}{2a^2}r\left|\frac{\epsilon^6}{a^6}\det E(v)\cdot\det n^\sigma(v)+\mathcal{O}\big(\epsilon^8\big)\right|^r\cdot$$
$$\cdot\frac{a^2}{2}\epsilon^{i_0 mn}\epsilon^{I_0 MN}\frac{E^a_m n^{M\sigma_0}_a E^b_n n^{N\sigma_0}_b}{\det E(v)|\det n^\sigma(v)|}\left(\frac{1+\mathcal{O}(\epsilon)}{\epsilon^2+\mathcal{O}(\epsilon^3)}\right). \tag{D.16}$$

What is left is taking the limit $\epsilon \to 0$ that we are ultimately interested in. Starting with the absolute value within (D.16), we realise

$$n^{J\sigma}_a\frac{\partial X^b_v}{\partial t^J} = \delta^b_a\operatorname{sgn}(\sigma)\left|\det\left(\frac{\partial X^c_v}{\partial t^K}\right)\right| \quad\text{and}\quad \det n^\sigma = \left|\det\left(\frac{\partial X^c_v}{\partial t^K}\right)\right|^2, \tag{D.17}$$

for $\frac{\partial X^a_v}{\partial t^J}$ being tangent vectors. As a consequence, we can formulate the limit $\epsilon \to 0$ of the absolute value within (D.16) as

$$\lim_{\epsilon\to 0}\left|\frac{\epsilon^3}{a^3}\sqrt{\det E}\,\left|\det\left(\frac{\partial X^c_v}{\partial t^K}\right)\right|\right|^{2r} = \frac{1}{a^{6r}}\left(\int_{\square_v}\mathrm{d}^3x\sqrt{\det E}(x)\right)^{2r} = \frac{1}{a^{6r}}V^{2r}_{R_x}, \tag{D.18}$$

based on the fact that $\epsilon^3\left|\det\left(\frac{\partial X^c_v}{\partial t^K}\right)\right| = \int_{\square_v}\mathrm{d}^3x$ for $\epsilon \to 0$.

For the remaining part of (D.16), which corresponds to $(p^-_{I_0 i_0})^{-1}$, we start by reformulating

$$\epsilon_{I_0 MN}n^{M\sigma_0}_a n^{N\sigma_0}_b = \det n^\sigma\frac{\operatorname{sgn}(\sigma_0)}{\left|\det\left(\frac{\partial X^d_v}{\partial t^K}\right)\right|}\epsilon_{abc}\frac{\partial X^c_v}{\partial t^{I_0}} = \left|\det\left(\frac{\partial X^d_v}{\partial t^K}\right)\right|\operatorname{sgn}(\sigma_0)\epsilon_{abc}\frac{\partial X^c_v}{\partial t^{I_0}}. \tag{D.19}$$

Using previous results and multiplying by an additional ϵ, we obtain

$$\lim_{\epsilon\to 0}(p^-_{I_0 i_0})^{-1} = \lim_{\epsilon\to 0}\left(\frac{a^2}{2}\frac{\epsilon\,\mathrm{sgn}(\sigma_0)\epsilon_{i_0 mn}\epsilon_{abc}\frac{E^a_m(v)E^b_n(v)}{\sqrt{\det E(v)}}\frac{\partial X^c_v}{\partial t^{I_0}}}{\epsilon^3\sqrt{\det E}(v)\left|\det\left(\frac{\partial X^d_v}{\partial t^K}\right)\right|}\right) \tag{D.20}$$

$$= \frac{\int_0^1 \mathrm{d}t \frac{1}{2}\epsilon_{i_0 mn}\epsilon_{abc}\frac{E^a_m E^b_n}{\sqrt{\det E}}\frac{\partial X^c_v}{\partial t^{I_0}}}{\int_{\square_v}\mathrm{d}^3x\sqrt{\det E}(x)} = \frac{2a^2}{\kappa}V^{-1}_{R_x}\int_0^1 \mathrm{d}t\left\{A^{i_0}_a(e(t)), V_{R_x}\right\}(\dot{e}^{\sigma_0}_{I_0})^a$$

$$= \frac{2a^2}{\kappa}V^{-1}_{R_x}\left\{\int_{e^{\sigma_0}_{I_0}} A^{i_0}, V_{R_x}\right\}. \tag{D.21}$$

Finally, combining both (D.18) and (D.20) with (D.3), we end up with

$$2\mathrm{i}\cdot\lim_{\epsilon\to 0} h^{i_0}_{I_0}\left\{\left(h^{i_0}_{I_0}\right)^{-1}, V^{2r}(R_{\square_\epsilon})\right\} = 2\frac{r}{2}\frac{2}{a^{6r}}V^{2r-1}_{R_x}\left\{\int_{e^{\sigma_0}_{I_0}} A^{i_0}, V_{R_x}\right\}$$

$$= \frac{1}{a^{6r}}\left\{\int_{e^{\sigma_0}_{I_0}} A^{i_0}, V^{2r}_{R_x}\right\} \tag{D.22}$$

and have therefore verified the identities (D.1) & (D.2).

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