Renormierung in der Schleifenquantengravitation

Renormalisation in Loop Quantum Gravity

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Abstract

In this thesis, we will investigate the quantisation ambiguities that arise during the canonical quantisation of General Relativity (GR), and we will develop a method of Hamiltonian renormalisation to fix the mentioned ambiguities.
"Quantisation" is an ansatz to obtain a fundamental (i.e. quantum) theory from a classical description. However, there is no way to "derive" this more complex framework if we only know a special case of it, i.e. its classical pendant. Hence, quantisation contains a lot of possible choices and must be supplemented by mathematical consistency and experimental evidence. In the case of gravity, whose effects are described by GR, no experiments are known which reveal properties of its quantum nature. Thus, we must rely purely on mathematical rigour to obtain a version of Quantum Gravity (QG). A promising candidate for this endeavour is "Loop Quantum Gravity" (LQG), a modern version of the canonical or Hamiltonian approach. During its development over the past 30 years, it achieved to describe a well-defined canonical quantum field theory. LQG presented a unique Hilbert space representation and the quantisation of constraints as operators acting thereon. During quantisation one must make certain choices by introducing "regularisation parameters". However, the details of the operators will be influenced by these choices even in the limit of vanishing regularisation parameters. Their varying physical predictions present an unsatisfactory situation as it is not clear which of those describe the real world.
The present work adapts the techniques from the covariant "renormalisation group" from Quantum Field Theory (QFT) to LQG. The philosophy of this machinery is that continuum theories should provide a consistent description, no matter with what resolution one looks at the system under consideration. This tool has been used in the context of defining other quantum field theories via the path integral framework. It turned out to be very successful and is, as of today, one of the main tools for studying weak and strong interaction in the Standard Model of particle physics. But, since the mathematical language of canonical QG is vastly different, we will translate the renormalisation group from covariant QFT. Afterwards, we will test it on a simple model, i.e. the massive free scalar field in arbitrary dimensions, and we will present a detailed analysis of it. This includes robustness of the fixed point under different choices of the renormalisation map and the fixed point's range of attraction. Also, we study properties of the discrete projections such as the perfect lattice Laplacian and restoration of continuum symmetries.
Finally, we will show the non-trivial impact of quantisation ambiguities in the context of LQG, which can already be seen in cosmological models describing our universe at large scales. Despite these drawbacks, the recent developments in the field allowed to pinpoint the caveats due to their mathematically precise formulation and suggest renormalisation techniques as a possible future improvement. It turns out that the new framework of direct Hamiltonian renormalisation serves as a good candidate to resolve the quantisation ambiguities plaguing QG.

Zusammenfassung

In dieser Arbeit werden wir die Wahlfreiheiten untersuchen, die während der kanonischen Quantisierung der allgemeinen Relativitätstheorie auftauchen, und werden eine Form von Hamiltonischer Renormierung entwickeln, um aus allen Wahlmöglichkeiten eine physikalisch sinnvolle Option zu isolieren.
Unter „Quantisierung“ versteht man den Prozess, aus einer klassischen eine fundamentalere (d.h. Quanten-)Theorie zu konstruieren. Da es jedoch keine Möglichkeit gibt, eine fundamentale Theorie aus einem ihrer Spezialfälle „abzuleiten“, folgt, dass die Quantisierung eine Menge an Wahlmöglichkeiten enthält (sogenannte „Quantisierungsambiguititäten“). Um die Quantentheorie zu finden, die die Natur korrekt beschreibt, würde man sich deshalb gerne an experimentellen Befunden orientieren. Im Fall der Gravitation, welche klassisch durch die allgemeine Relativitätstheorie beschrieben wird, sind bis heute keine Experimente bekannt, die uns etwas über ihre Quantennatur verraten. Folglich muss man sich vollständig auf mathematische Rigorosität verlassen, um einen Kandidaten für Quantengravitation zu erhalten. Ein vielversprechender Ansatz ist die „Schleifenquantengravitation“ (auf Englisch *„Loop Quantum Gravity“* (LQG)), die eine moderne Version des kanonischen, oder auch Hamiltonischen, Zugangs darstellt. Während ihrer Entwicklung in den vergangenen 30 Jahren, ist es gelungen aus ihr eine wohldefinierte Quantenfeldtheorie (QFT) zu konstruieren, die eine eindeutige Hilbertraum-Darstellung beinhaltet. Die Quantisierung der auftretenden Zwangsbedingungen wird durch Operatoren auf diesem Hilbertraum realisiert. Bei der Quantisierung müssen Regularisierungswahlen getroffen werden, die auch im Limes eines verschwindenden Regulators die Details der Operatoren beeinflussen. Damit unterscheiden sich die Operatoren in ihren physikalischen Vorhersagen und man befindet sich in einer unangenehmen Lage: Ohne Experiment ist nicht klar, welche Wahl die Realität wirklich beschreibt.
Die vorliegende Arbeit adaptiert das erprobte Verfahren der kovarianten „Renormierungsgruppe“ aus der QFT für die LQG. Die zugrunde liegende Philosophie des Verfahrens ist die Folgende: Eine Kontinuumstheorie soll eine konsistente Beschreibung haben, unabhängig von der Auflösung unter der sie betrachtet wird (d.h. unabhängig davon, wie fein das zugrunde liegende Raumzeit-Gitter ist). Diese Maschinerie wurde mit großem Erfolg auf anderen Gebieten angewendet, insbesondere bei der Definition von Quantenfeldtheorien mittels des Pfadintegral-Formalismus. Bis heute ist es eines der wichtigsten Werkzeuge, um sowohl die schwache, als auch die starke Wechselwirkung im Standardmodell der Elementarteilchenphysik zu untersuchen (z.B. „Lattice QCD“). Jedoch sind die mathematischen Methoden, mit denen die Renormierungsgruppe ursprünglich beschrieben wurde, sehr unterschiedlich von denen, die man in der kanonischen Quantengravitation verwendet. Deswegen werden wir dieses Verfahren entsprechend „übersetzen“, um es in jenen physikalischen Systemen anwenden zu können, welche durch eine Hamiltonfunktion beschrieben werden. Anschließend werden wir unsere neue Formulierung der Renormierungsgruppe in einem einfachen Modell testen, explizit einem massereichen, freien Skalarfeld in beliebigen Dimensionen, und eine detaillierte Analyse hiervon präsentieren. Dies beinhaltet die Stabilität des Fixpunktes und seines Attraktionsgebietes gegenüber Veränderungen der Renormierungsabbildung. Darüber hinaus betrachten wir Eigenschaften der diskreten Theorien, wie den perfekten Gitter-Laplace-Operator, und stellen fest wie Symmetrien des Kontinuums wiedergefunden werden können.
Zum Abschluss werden wir zeigen, dass in der LQG diese Quantisierungsambiguitäten tatsächlich nicht-trivialen Einfluss haben, indem wir ein kosmologisches Modell untersuchen, welches unser Universum auf großen Skalen beschreibt. Dank der vorangegangen Fortschritte auf dem Gebiet und ihrer mathematischen Präzision, auf denen diese Arbeit aufbauen konnte, ist es möglich, die übriggebliebenen Lücken aufzuzeigen, die auf natürliche Weise die Renormierungsgruppe als Technik für weitere Verbesserungen vorschlagen. Es stellt sich heraus, dass das neue Verfahren der direkten Hamiltonischen Renormierung einen guten Kandidaten darstellen könnte, um das Problem der Quantisierungsambiguitäten zu lösen, die die Quantengravitation plagen.

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Kapitel I

Introduction

I.A Motivation and Historical Review

There are two topics in theoretical physics which spread their influence far afield and are known to most people even outside the physics community. These are the "Theory of Relativity" developed by Einstein on the one hand and "Quantum Theory" on the other hand. Their publicity is partially due to their predictions, which drastically changed our way of perceiving the world, and the enormous accuracy with which both have been verified by experiment.

That our world in the microcosm is fundamentally quantum was discovered over 100 years ago, starting with the discovery of the Planck constant h [1, 2]. Its very early success was the explanation of many aspects of molecular physics [3–7] and the correct prediction of new quantum degrees of freedom such as spin [8–10]. It features, however, even more bizarre phenomena, such as the fact that it is no longer predictive. In contrast to a classical theory, we are forced to accept that we can only give probabilities for what happens to a particle after we have measured it as accurately as possible (which, due to the famous Heisenberg uncertainty obstruction, can never be without error bars [11]). Today, quantum theory is of use in numerous applications, e.g. in detection methods like nuclear magnetic resonance, for which numerous Nobel prizes have been awarded [12–14].

Almost in parallel, Einstein initiated in 1915 a revolution of our understanding of space and time [15, 16]. With General Relativity (GR), he found a geometric interpretation of the gravitational field which answered many questions plaguing astronomers back then. As the field evolved, people were able to use GR to predict the collapse of stars forming black holes [17–19] as well as gaining first insights into what happened in the beginning of our universe [20–32]. The idea of the "Big Bang" was born, which roughly states that the universe started as a single, infinitesimally small point called singularity. Even more, GR has found its application in our everyday life, as without its predictions of the gravitational redshift [33], the global positioning system (GPS) used for navigation would not work nearly as precise as it does today.

Despite the huge success of both theories, they are fundamentally very different as they describe our world at completely opposite scales. Each also features its own drawbacks: Quantum Field Theory (QFT) is written in a mathematical language which does not even allow the presence of gravitational fields as described by GR. Moreover, the mathematical description of QFT in four spacetime dimensions has not yet been completed. Currently, the only way to describe scattering theory is by a perturbation series, which however does not converge [34–37]. However, GR does not fare better as it predicts its own failure: Penrose and Hawking discovered that the origin of our universe from an initial singularity is unavoidable in this classical theory [38–40]. But if everything collapses into a single point then the matter energy density becomes infinite in this point. This implies that GR leaves its domain of validity and must be replaced by a more fundamental theory.

This "fundamental theory" is as of today unknown. However, by our understanding, it should be a merger of Quantum Theory and GR. This is the starting point for the search for a theory of *Quantum Gravity* (QG).

In the 1930s, Dirac started with attempts to unify quantum theory at least with the principles of Special Relativity [41–45] and was shortly followed by Pauli, Jordan and Heisenberg [46, 47]. And while in the following years people were able to make progress via the invention of renormalisation on the conceptual side, the establishment of a non-perturbative quantum field theory in four spacetime dimensions remains elusive to this day. However, following the framework of canonical quantisation developed by Dirac back then, a modern approach to QG originated in the last decades:

The field of "Loop Quantum Gravity" (LQG) (cf. [48–52] for a general introduction) started primarily with the discovery of the nowadays famous Ashtekar variables in 1986 [53–55]. His work was based on the ADM or Hamiltonian formulation of four-dimensional GR, which turned out to feature an involved constraint algebra [56], including a complicated, non-polynomial scalar constraint, which captured the dynamical content. Extending seminal work by Sen [57–59], Ashtekar (and later Barbero [60, 61]) succeeded in rewriting this Hamiltonian formulation in such a way that they were able to use the machinery for "Quantisation of Gauge Theories" which had already been hugely successful in the past for describing the weak and strong interaction [62–65]. Indeed, exactly like the weak interaction, the Ashtekar-Barbero variables were based on the compact structure group $\mathrm{SU}(2)$ which enabled a mathematically rigorous construction of a kinematical Hilbert space equipped with operator constraints. The Ashtekar-Isham-Lewandowski representation [66, 67] of the algebra of elementary operators, called holonomy-flux algebra, implemented two of the three constraint types and was later shown to have suitable uniqueness and irreducibility properties [68–73].

In 1996, Thiemann was the first to give a possible completion to the program of canonical quantisation by constructing a well-defined representative of the scalar constraint [74, 75] . This was the starting point for various applications such as black holes in LQG [76–79] or the application to cosmological models of GR. The latter runs under the name of Loop Quantum Cosmology (LQC) and it presented a possible resolution of the Big Bang singularity for the first time [80–85].

However, the setup for full LQG was not fully satisfactory. Namely, the quantisation of the scalar constraint by Thiemann involved several choices of regularisation steps, which leave an imprint in the details of the final operator as the regulator is removed. Of course, these details have an impact on the physical predictions of the theory. Hence, one should also consider other regularisation proposals, foremost some for which the algebra of constraints for GR closes. To deal with complications arising from the latter, the master constraint programme [86–91] was developed and later refined in Algebraic Quantum Gravity (AQG) [92–95], which suffers from fewer quantisation ambiguities.

Due to the latter fact, the analogy to Lattice Gauge Theory [96–99] was maximal and one could hope to use tools from there to fix the quantisation ambiguities.

We are especially referring to the covariant and background dependent "renormalisation group". This method was pioneered in 1954 by Gell-Mann and Low [100] and in 1966 by Kadanoff's block-spin transformation [101]. Later Wilson applied it to critical phenomena winning him the Nobel Prize in physics in 1982 [102–105]. The renormalisation group has shown promise in describing the physics of strongly interacting many-body systems, where different phase transitions occur, and in statistical physics when one deals with various scaling relations and critical indices [106–114].

In contrast to this, the application we have in mind is vastly different, as GR is background independent. But, as the formulation of the renormalisation group in the literature has made crucial use of the background metric, it is pivotal to redefine its structure to make it applicable for the context of fixing the quantisation ambiguities of QG.

First steps in this direction were taken in the "Asymptotic Safety" programme, developed by Weinberg, Reuter, Saueressig and Percacci [115–119]. Here, the idea was to formulate renormalisation conditions in a background independent situation and search for its fixed point. Parts of those ideas are also realised in the programme of "Causal Dynamical Triangulations" of Ambjorn, Loll, Jurkiewiz and Smolin [120–122]. However, the Asymptotic Safety programme as well as Causal Dynamical Triangulation are formulated in terms of path integral measures, while most of the work in LQG is in the Hamiltonian setting (see [123–127] for the state of the art in the path integral formulation of LQG). Thus, in its application to LQG it would be desirable to have the renormalisation group in a Hamiltonian formulation.

Of course, this shorthand exposition of QG cannot be comprehensive and many important aspects were left unmentioned. For further references we suggest the following sources: [48–52].

I.B Overview of the Results

The starting point of this thesis was the unsettling situation in Quantum Gravity, as well as in other constructive Quantum Field Theories, that a lot of ambiguities arise during the process of quantisation. This is especially worrisome for Quantum Gravity as until today no experiments are known that could help us to eliminate these quantisation ambiguities. However (as this thesis will show), these choices have drastic influence on the physical predictions.

Despite this, the canonical approach known as "Loop Quantum Gravity" has over the last decades evolved into a promising candidate for Quantum Gravity. It presents rigorously defined candidates for a Hilbert space, on which the elementary phase space variables are quantised in terms of operators, as well as for a Hamiltonian operator, which captures the dynamical content. It is hence the next logical step to determine among all the possible candidates a unique choice whose predictions can be trusted. Some steps towards this direction been tackled in this thesis, and build on the earlier, mathematically precise developments in LQG due to which a

possible strategy to resolve these ambiguities suggested itself.
The mentioned strategy to deal with these kinds of ambiguities is used in the covariant approach towards Quantum Field Theories and is known as "Renormalisation". This is a procedure which determines on a discretised system a measure such that it behaves as a consistent projection of the continuum measure to some finite resolution. The machinery of renormalisation has proven very successful in eliminating quantisation ambiguities and thus one would want to apply it to the problems in canonical Quantum Gravity.
However, as the canonical and the covariant approach are very different from the onset, it is obvious that the covariant renormalisation procedure could not be straightforwardly used for Loop Quantum Gravity. This thesis extends earlier work in this direction to formulate a version of renormalisation which stays completely in the Hamiltonian setting. This is the "direct Hamiltonian renormalisation", which has been thoroughly tested and verified for the toy model of the free, massive scalar field. This strengthens the hope that renormalisation is a way to investigate (and some day hopefully fix) the quantisation ambiguities in Loop Quantum Gravity, such that the reliability of its physical predictions can be confirmed.

The subject of this thesis was suggested by Thomas Thiemann. In collaboration with him and Thorsten Lang the direct Hamiltonian renormalisation was developed in [128–131]. In a joint project with Andrea Dapor the expectation values of Hamiltonian operators in cosmological coherent states were found to be prone to the ambiguities of a chosen regularisation in [132, 133]. These results inspired a numerical investigation in the context of LQC together with Mehdi Assanioussi, Andrea Dapor and Tomasz Pawłowski in [134].

Chapter II : Quantum Field Theory - In this chapter, we revisit the established strategy of constructive QFT to obtain a quantum version of any classical canonical theory. Due to the involved nature of a field theory, the several ambiguities which occur during the process of quantisation get even worse. Having infinitely many different, inequivalent states to choose from is aggravated further by the fact that, up to today, not a single interacting example for a QFT in four spacetime dimensions is known. To get more control over the various ambiguities, we study the broad ideas of path integral quantisation and compare the possible choices of a measure of spacetime fields with the ambiguities which arise during quantisation in the Hamiltonian framework. This is partially achieved via the Osterwalder-Schrader reconstruction [135–137].
In this work, we will generalise the Feynman-Kac proposal [138, 139] for defining path integral measures. This will result in a reverse procedure to the Osterwalder-Schrader reconstruction - the Osterwalder-Schrader construction -, which builds a covariant quantum theory out of every suitable canonical quantum description. Indeed, we can show that under certain technical assumptions both processes are inverses.
The advantage of having Osterwalder-Schrader bijection explicitly at hand is that we can now relate ambiguities in both the canonical and the covariant framework with each other. So, while no scheme is intrinsically favoured in terms of uniqueness, we can now hope to translate strategies which use in one formulation to fix the quantisation ambiguities to the other. Hence, this can also be regarded as a prerequisite for the next chapter.

Chapter III : Renormalisation - In this chapter, we recall the renormalisation group in the covariant formulation in which it was originally invented. Given a cylindrically consistent coarse graining map, one would have to look for a fixed point of the flow of the block spin transformation corresponding to the coarse graining map. This flow must be started with the initial discretisation of a path integral measure which agrees with the full covariant theory in its continuum limit. One must take note, that the fixed point family itself is not a fundamental theory, but rather are the cylindrically consistent projections from an underlying continuum theory [140–146].
This thesis will achieve to transfer the renormalisation prescription to the Hamiltonian level by using the developed Osterwalder-Schrader bijection. A procedure following exactly the flow of the reconstructed data from a covariant measure will, however, require the computation of the spacetime measure at each intermediate step. To circumvent this, we introduce an alternative (yet maximally close) renormalisation group flow: the direct Hamiltonian renormalisation. We then study both schemes in the test case of the massive, free scalar field in arbitrary dimensions and find that both their fixed points agree in the continuum limit. However, we will see that it is the fixed point of the direct Hamiltonian renormalisation which displays the finite resolution matrix elements of the continuum Hamiltonian.
Afterwards, we investigate properties of the latter renormalisation flow: first, we verify that the flow indeed drives the initial discretisation into the fixed point, in other words, it is an attractive fixed point. This holds also true when considering different initial discretisations if they agree in their continuum limit. This is an important property as it guarantees that we do not have to be careful which ambiguous discretisation to pick in the beginning. We then look at different choices for the coarse graining map, other cylindrically consistent choices as well as some which are not. We see that those which do not satisfy this criterion - albeit being considered in the literature - lead to fixed points which cannot be understood as projections from the conti-

nuum. However, other consistent block-spin transformations lead to the same physically sensible fixed point, indicating that our more restrictive framework captures important physical insight.
From this fixed point theory, we can extract the perfect Lattice Laplacian for the massive free scalar field, i.e. a difference operator which possess all the important properties of its continuum counterpart. We find that it is no longer a local operator, but that its excitations get exponentially suppressed the longer the lattice distance is. Lastly, we show how symmetries of the continuum, such as rotational invariance, can be found in the cylindrical projections at finite resolution. We determine a criterion for the rotational invariance of a lattice theory and study it numerically for the aforementioned test case.
This thorough analysis is essential to confirm that the direct Hamiltonian renormalisation leads indeed to reliable theories. Due to the results obtained here we can trust the scheme and hope to apply it for Quantum Gravity, which is also prone to troublesome quantisation ambiguities.

Chapter IV : General Relativity - In this chapter, we outline the basic idea behind GR and its application in cosmological models. Historically, GR was first formulated in terms of the Einstein-Hilbert action i.e. in a covariant framework. It was only in 1960 that a Hamiltonian version was discovered in the ADM formulation. We repeat their construction and proceed further to the Ashtekar-Barbero variables and later on the holonomy-flux algebra, which will be suitable for developing a theory of QG. The dynamical content is expressed in terms of several constraints, one of them is the so-called scalar constraint. In the presence of a suitable dust or clock field it can be associated with a physical Hamiltonian driving the dynamics [147–153]. We revisit the most prominent approximation to the aforementioned scalar constraint in terms of holonomies and fluxes.
Then, we turn towards the cosmological sector of GR, i.e. the Robertson-Walker metric, and for the first time compute the value of the complicated constraint on a discrete set of holonomies, namely a cubical graph. We investigate its difference to the standard continuum value and realise that its dynamics replaces the initial singularity with a Big Bounce.
However, as different regularisations produce different predictions of what has happened before the Big Bounce, we conclude that in canonical Quantum Gravity it will become important which choice to pick.

Chapter V : Loop Quantum Gravity - We repeat the programme of canonical quantisation for the gravitational field in the way it is envisioned in LQG. We comment on the unique, diffeomorphism invariant state which is a representation of the holonomy-flux algebra. In this Hilbert space, a representation of the group $\mathrm{SU}(2)$ labels each path and it is possible to construct coherent states peaked on classical holonomies and fluxes for the mentioned path (and an associated surface) [154–158]. Then, we repeat how certain geometric operators such as the volume can be quantised and how the Gauss and the spatial diffeomorphism constraints are implemented. We look also at the regularisation Thiemann proposed, which can be used to define a quantum scalar constraint operator.
Following this, we investigate this constraint operator for its quantisation ambiguities by testing it on a coherent state peaked on semi-classical Robertson-Walker spacetime. We find explicit formulas for the expectation value including first corrections in $\hbar$. However, its physical predictions are still affected by the quantisation ambiguities: by computing the expectation value of the scalar constraint, we arrive at an effective Hamiltonian from the full theory. However, when choosing different details in the regularisation we find different physical predictions, especially in the way a Big Bounce resolves the initial singularity.
This finishes our claim that the quantisation ambiguities in LQG have significant impact and must be resolved before any reliable predictions can be made. However, the earlier, mathematically rigorous developments were crucial in order that one now can identify strategies of future improvement, i.e. renormalisation techniques. One possible incarnation thereof has been formulated in this thesis: the direct Hamiltonian renormalisation.

Chapter VI : Conclusion and Outlook - Here, we summarise our results and finish with a list of topics for further research following these results.

At the beginning of each chapter, we will give a brief overview over the content. It will summarise the key concepts and main results obtained in the remaining sections.

Kapitel II

Quantum Field Theory

The necessity for a quantum description of the world surrounding us is rooted in a number of historical discoveries in the late 19th and early 20th century, most notably the problem of black body radiation [2, 3] and the photoelectric effect [4, 5]. It transpired that our *classical* point of view of the world must be considerably changed. Instead of particles and ordinary fields (e.g. electro-magnetism), the fundamental building blocks of the universe must obey strange and - back then - unknown properties on very small scales. Since the beginning of the 20th century, physicists have tried to develop a mathematical framework by which this new nature could be described [6, 7, 11, 34–37, 41, 65, 159–162] - a process that is still developing today!
In this chapter, we will revisit some of the many viewpoints which physicists adapt today when trying to define a mathematically rigorous framework to describe the quantum nature of fields with non-trivial interaction. However, we will see that this task is not yet completed: there is *no* four-dimensional quantum theory fulfilling all the physically plausible criteria we intuitively want an interacting field to have.[1]
In this chapter, we will, for pedagogical reasons, treat the spacetime field of the metric as the flat Minkowski metric $\eta_{\mu\nu}$. As will be shown in chapter *IV. General Relativity*, one can see that this metric field corresponds to the solution of the Einstein field equations for empty (i.e. matter free) space. Of course, this is an approximation, which is *necessarily* wrong as soon as massive particles and fields come into play. But the effects of the gravitational field are of such a low order of magnitude that, in a first approximation, it is assumed to be safe to ignore them. We will come back to integrate the full gravitational interaction in the last chapter of this thesis. For the moment, however, this puts us into the advantageous position that we can use the concept of *imaginary time*. It is a mere mathematical trick to perform a Wick rotation $t \to i\beta$ in order to remove the minus sign in the time component of $\eta_{\mu\nu}$. In other words, we move from Lorentzian to Euclidian signature $(+, +, +, +)$, which allows us to treat space and time on an equal footing. Apart from rendering computations easier, this does not serve any physical purpose and at the end of the day we will always "rotate back" to real time.

In order to start tackling the problem of defining a "quantum theory" of fields (or particles), we have to think about classical field theory for a moment. This is a well-understood concept and we of course want to regain it once all the scales involved in our experiments are sufficiently large. This "quantum to classical" transition is a necessary feature, as our everyday world appears to be manifestly classical.
In the following, we will adapt an algebraic point of view. As this is slightly different from the usual terminology, we will carefully define the most important concepts. First, we envision a classical field theory as follows: the result of any experiment must depend on the configuration variables of the system. The space of all possible combinations of degree of freedom which the system can be found in at a given instant of time t is known as the *phase space* $\mathcal{F}$. For the moment, we will talk about field theories in their Hamiltonian formulation. Then, for each field species, the phase space consists of the configurations of the field $\phi(\vec{x})$ itself and of those of its canonical momentum $\pi(\vec{x})$. The result of any measurement will be some function $f : \mathcal{F} \to \mathbb{C}$ from this phase space to the (complex) numbers, i.e. the pointers of the measurement device. Thus, the set of all measurements we could perform is the space of all such smooth functions, which we denote by $C^\infty(\mathcal{F})$. A *theory* (classical or quantum) is now merely a prescription of which result a measurement is supposed yield. We want to emphasise this: given the phase space point which the system occupies, the theory predicts the average result for any measurement. Hence, in mathematical terms, a theory is described by a *state* which

[1] These criteria run under the name of *Wightman axioms* [163] and, in fact, the Clay Mathematics Institute has offered one of its millennium prizes for a concrete formulation of a Yang-Mills QFT [164]. This drawback is countered by the astonishing fact that the unfinished formulations used today provide excellent agreement with the experiments, e.g. Quantum Electrodynamics (QED) is verified within ten parts in a billion [165].

maps observables onto their expected outcomes:

$$\omega \;:\; C^\infty(\mathcal{F}) \;\to \mathbb{C}\,. \tag{II.1}$$

This formulation, as yet very formal, can be applied to a practical problem by giving a concrete form to ω so that actual calculations can be performed. This is indeed possible by making contact to the framework of functional analysis and representation theory, hence we must familiarise ourselves with these concepts in section *II.A. Mathematical Background.*[2]

Imagine that at time t you have $z = (\phi, \pi) \in \mathcal{F}$, then a very simple choice for ω is just to perform each experiment on the mentioned field. Precisely speaking: one evaluates each observable $a \in C^\infty(\mathcal{F})$ on the given point in phase space z, such that $\omega(a) = a(\phi, \pi)$. This specific choice of ω_z for each $z = (\phi, \pi)$ corresponds to our classical point of view. For example, it implies that $\forall a, b \in C^\infty(\mathcal{F})$ we find

$$\omega_z(ab) = \omega_z(a)\omega_z(b)\;. \tag{II.2}$$

Thus, we have vanishing correlation functions. In other words, ω_z predicts an exact outcome of the experiment not just the average, i.e. there is no variance! Hence, from a classical point of view this choice of a theory works very well.

However, we already know from experiments that there are corrections to the classical world on very small scales. For these quantum contributions we will introduce a new parameter, which is called the *(reduced) Planck constant* $\hbar$.[3] The idea is that all deviation from the classical theory must be proportional to $\hbar$. However, the exact form of the deviation is to be determined by comparing it to experiments. Here it is found that in the deep quantum regime the property of predictivity is lost!

Even if all information of the system is available, the outcome of a measurement cannot be predicted beforehand. As mentioned before, this is connected to a property of the state and to the product of two observables. Hence, a quantum theory in agreement with the experiment must be such that (II.2) is lost. A possible way to achieve this is to define a new product on the algebra $C^\infty(\mathcal{F})$ which is non-commutative and implies that the two observables are no longer independent of each other. How to choose this new product presents a certain ambiguity only restricted by the condition that the deviation from the normal product should vanish if $\hbar$ is sufficiently small. A possible choice is thus the following product on the space of all observables:

$$a \star b \;:=\; a\cdot b \,+ \frac{i\hbar}{2}\,\{a,b\}\;, \tag{II.3}$$

where $\{\cdot,\cdot\}$ stands for the Poisson bracket of the system. It is important that the joint measurements of two (or more) elements now depend on the order in which we they appear. However, this is not a property of the above given example for a state ω, hence we have indeed a distinguishing criterion between classical and quantum theories.

In section *II.B. Canonical vs Covariant Quantisation*, we will see that nonetheless there is a way to give a concrete form to ω for a quantum theory, in form of a *representation* of the algebra of all possible observables. By this we mean that we want to assign to every element a in $C^\infty(\mathcal{F})$ (say every experiment we want to conduct) an element $\hat{a} \in (C^\infty(\mathcal{F}), \star)$, which we equip with an involution $\hat{a} \mapsto \hat{a}^*$. We will see later that, moreover, each $\hat{a}$ is in correspondence with a self-adjoint operator $\pi(\hat{a})$, which is a map on some (infinite dimensional) Hilbert space $\mathcal{H}$. This is well-motivated, as in general the ordering matters when considering operators. Their non-commutativity is described by the commutator, motivating the assignment $i\hbar\{\cdot,\cdot\} \to [\cdot,\cdot]$ while $a \to \hat{a}$. We will call this assignment $\hat{}\;:\; C^\infty(\mathcal{F}) \to (C^\infty(\mathcal{F}), \star)$, however its implementation is not possible in general: the Groenewold-van Hove theorem [167, 168] is a mathematical proof stating that there is *no* consistent mapping $\hat{}$ such that $\hat{a}\star\hat{b} = \widehat{ab}$ and $\hat{\bar{a}} = \hat{a}^*$ hold for all $a, b \in C^\infty(\mathcal{F})$ with the non-commutative product from (II.3). In other words, we cannot demand this assignment on the whole space of observables, but only on a subset, which we have to choose manually. This of course introduces other ambiguities during the process of developing the quantum theory. Choosing one of these ambiguities corresponds to considering specific maps $\hat{}$ into a $*$-algebra $\mathcal{A}$, which we generate from the chosen subset. Often, one referees to $\hat{}$ as *ordering prescription*. E.g. "Weyl ordering" means that a polynomial in ϕ, π $a \in C^\infty(\mathcal{F})$ is mapped to its the total symmetrisation in $\mathcal{A}$.

Once the assignment has been chosen and the quantum algebra of observables $\mathcal{A}$ has been constructed, one is faced with the question of how to choose the correct state ω. We remember that in the classical case

[2] During this chapter we will require basic knowledge of differential geometry. The reader unfamiliar with it, is refereed to section IV.A of chapter *IV. General Relativity*, which is self-consistent and be read in advance if necessary.

[3] This tiny object is one of the most accurately measured constants [166] with value $\hbar \approx 1.0546 \cdot 10^{-34}\,\mathrm{J}\cdot\mathrm{s}$ and tells us about the quantum nature of the system under investigation. Hence, in the limit $\hbar \to 0$ we would not measure any quantum effects at all and call it thus the *semi-classical limit*.

we had one state ω_z for each point z in phase space. Similarly, there is a huge abundance of possible quantum systems we could encounter and in general we should aim at finding a suitable state for each possibility. An special subclass among them, are those states, which reassemble the classical states ω_z in the following way: for a given observable $a \in C^\infty(\mathcal{F})$ (or a set of them) the predictions of the quantum state on $\hat{a}$ agree with those of ω_z on a up to corrections of order $\hbar$. This is a possible definition for a *semi-classical* or *coherent state*. However, upon demanding further properties, e.g. that the deviations stay of order $\hbar$ even for the whole time evolution of the observables, it can become an increasingly hard task to find such (stable) coherent states in general.
But, one can at least classify the set of all possible quantum states: Gel'fand, Naimark and Segal found a construction [169, 170] by which any state on a (unital) algebra $\mathcal{A}$ becomes equivalent to the expectation value of a representation of $\mathcal{A}$ on a specific vector of a Hilbert space, which is commonly called the *vacuum vector* Ω. If the state is invariant under global time translations, this is a well-motived terminology, as Ω has then the generic property to be annihilated by the operator $\pi(\hat{H})$ that is the generator of time translations. This means in explicitly: Let α_t^H be the flow that evolves any observable at time 0 to its pendant at time t. Then, any state ω_0 that fulfils

$$\omega_0(\alpha_t^H(\hat{a})) \;=\; \omega_0(\hat{a})\;, \qquad\quad \forall\, \hat{a} \,\in\, \mathcal{A}\,. \tag{II.4}$$

will give rise to an element Ω with $\pi(\hat{H})\Omega = 0$. And as we envision the classical vacuum to be invariant under time-shifts (if there is no field which evolves the system will remain unchanged), this element is called *vacuum vector*.
However, up to today there has *not* been found *any* state ω_0 for an interacting Hamiltonian in four spacetime dimensions! But as everything in the real world interacts with its surroundings, this is an important problem to deal with.[4]

Although this approach - commonly referred to as *constructive QFT* - seems to have in a certain sense fail so far, there is also another approach towards defining an interacting QFT, which at first glance differs quite drastically from the outlined framework. This second approach is known as covariant or *path integral* quantisation.
The starting point is once again a classical (field) theory. Instead of observables at a given instant of time, one considers observables in spacetime. These are consequently functions of the history fields $\Phi(\beta = -it, \vec{x})$, i.e. a collection of fields at every instant of time. Since the space of functions allowed this way has become even bigger, we will give a new name to the corresponding map from spacetime observables F to the complex numbers, which are the outputs of an experiment: The *path integral measure* μ is defined heuristically as

$$\mu(\,F\,) \;=\; \int d\mu(\Phi) F(\Phi)\;, \qquad d\mu(\Phi) := \;\mathcal{D}\Phi \; e^{-S[\Phi]/\hbar} \tag{II.5}$$

wit $\mu(1) = 1$ and where $S[\Phi]$ is the action of the corresponding classical interacting theory. The path integral measure consists of $\int \mathcal{D}\Phi$, which denotes integration over *all* possible field configurations; an object to which a priori one cannot give a rigorous mathematical meaning!
One should pay attention to the fact that this is a mere guess for a possible framework by which to formulate a quantum theory. Hence, the question arises whether it is equivalent to one of the possible choices which we encountered during the aforementioned canonical approach. Also, it is not clear if there exist slight alterations to the proposal (II.5) to account for the other ambiguities. Due to $d\mu(\Phi)$ being an undefined object in its full generality, it is hard to study how different choices might alter the predictions of the quantum corrections and maybe introduce the same amount - or worse - of arbitrariness as in the canonical framework. In order to answer this question, one would need to find a way to compare both methods for defining a quantum theory and try to construct a map between them. Half of this was achieved in 1973 by Osterwalder and Schrader [135–137] by constructing a canonical theory from every well-behaved measure. We will see that also the converse statement is true: from any suitable canonical theory one can construct a measure, as has been done in [128] based on ideas from [138, 139]. This will be the topic of the section *II.C. Bijection between OS measure and OS data*. Let us outline the general strategy of both procedures:
Assume, we have a measure μ from the space of history fields Φ (and hence a definition of a possible quantum theory). We want to reformulate this in a language where we have a concrete Hamiltonian operator $\hat{H}$ (in an abuse of notation we identify $\pi(\hat{H})$ with $\hat{H}$ in the following) at hand that evolves a configuration of the

[4] Although one could construct states for interacting field theories in lower spacetime dimensions, in 4D one has only managed to find states for the free scalar field and the free Maxwell field. It might be tempting to just use the corresponding *free vacuum vectors* for computations in interacting theories, however Haags No-Go theorem forbids implementing any interacting Hamiltonian on the Hilbert space obtained from the aforementioned free vacuum vectors [171, 172].

quantum field, which is described by some element in a Hilbert space $\mathcal{H}$. If $\mathcal{H}$ features also a vector that does not change under time evolution, we will call it the vacuum vector $\Omega \in \mathcal{H}$. Since the Hamiltonian generates translations in time, it shall hold $\hat{H}\Omega = 0$. This triple $(\hat{H}, \mathcal{H}, \Omega)$ will be called Osterwalder-Schrader data (OS data) in the following and it turns out that one can always find it, provided the spacetime measure μ obeys certain properties known as the Osterwalder-Schrader axioms (or even a subset thereof[5]).
We consider the space of some bounded observables, i.e. functionals $\Psi(\Phi)$ from the history fields $\Phi(\beta, \vec{x})$ to $\mathbb{C}$ that only read $\Phi(\beta, \vec{x})$ at positive times $\beta > 0$. A key idea from Osterwalder and Schrader was to introduce the *time reflection* operator R and consider the subspace of those Ψ for which

$$\langle \Psi, \Psi' \rangle_{\mathcal{V}} \geq 0 \qquad \text{with} \qquad \langle \Psi, \Psi' \rangle_V := \int d\mu(\Phi)\, \overline{\Psi(\Phi)} (R\Psi')(\Phi) \tag{II.6}$$

Herewith the construction of a Hilbert space was possible, whose elements are the equivalence classes with respect to the Null space of (II.6). In other words, we have brought together all elements which differ from each other by some element of norm zero. These equivalence classes will be called $[\Psi]$, with some arbitrary representative Ψ. As Ψ is still a functional of $\Phi(\beta, \vec{x})$, we can define a *time-shift operator* $K(s)$ on it, which will simply force the functional to read the history field at $\Phi(\beta + s, \vec{x})$. Then we simply define the Hilbert space as all possible equivalence classes and the Hamiltonian as the generator of the time-shifts:

$$K(s) \;=:\; \exp(\, -s\hat{H}\,)\,, \qquad \mathcal{H} \;:=\; \overline{\text{span}(\,\{[\Psi]\}\,)}\,, \qquad \Omega \;:=\; [1]\,, \qquad \langle [\Psi], [\Psi'] \rangle_{\mathcal{H}} := \langle \Psi, \Psi' \rangle_V . \tag{II.7}$$

This is the punchline of the famous Osterwalder-Schrader reconstruction.[6]
Now assume the situation were reversed and we would have given the OS data $(\hat{H}, \mathcal{H}, \Omega)$ but wanted to have a spacetime measure μ at hand. This measure is supposed to give us a measurement prediction for each possible spacetime observable. We consider a generator of this set, namely the spacetime-dependent *Weyl elements* $W[F]: \;\Phi \mapsto W[F](\Phi)$ with smearing functions F. If it can be written as a product of some purely spatial, bounded observables $W[f_k, \beta_k]$ at sharp times $\beta_k > \beta_{k-1}$, then we simply define the measure to be

$$\mu(\, W[F]\,) \;=\; \mu(\,\prod_k W[f_k, \beta_k]\,) \;=\; \langle \Omega\,,\; \hat{w}(f_N)\, e^{(\beta_N - \beta_{N-1})\hat{H}} \,...\, e^{-(\beta_2-\beta_1)\hat{H}}\; \hat{w}(f_1)\, \Omega \rangle_{\mathcal{H}}\,, \tag{II.8}$$

where $\hat{w}(f)$ are the spatial Weyl elements, bounded operators on $\mathcal{H}$. After a lengthy calculation, it is shown that μ defined this way also satisfies the necessary and physically sensible Osterwalder-Schrader axioms. Afterwards one is free to move arbitrarily between both formulations as we will show that both maps are inverses of each other.[7]

Another important lesson to learn from this is that the ambiguities during the quantisation process in the canonical approach are equivalent to the ambiguities in the definition of the path integral measure. But while there are no trade-offs in the principal freedom of constructing QFTs, both methods so far fail at presenting one single non-trivial interacting example in 4D.
As mentioned, in 4D the only example where both approaches could be carried out rigorously and indeed shown to yield the same consistent result, is the case of the *free field*. Hence, to make the hugely abstract method of quantisation more understandable, we will at the end review both constructions and how to interchange between them, in the section *II.D. Example: Free scalar field* which follows closely [128].

We finish this introduction with a very quick summary of the steps of canonical quantisation as discussed above. As this programme was first suggested in [42–45], it is commonly known as the *Dirac programme of canonical quantisation*:

1. Choose a set $\mathcal{E}$ of observables, e.g. the classical phase space variables of the theory
2. Find a representation thereof as operators in an (auxiliary) Hilbert space $\mathcal{H}_{kin}$ satisfying the standard commutation relations, i.e. $\{.,.\} \to -i/\hbar[.,.]$
3. If present, promote the constraints to (self-adjoint) operators in $\mathcal{H}_{kin}$. The space of solutions, i.e. elements in the kernel of all constraints, defines the physical Hilbert space $\mathcal{H}_{phys} \subset \mathcal{H}$

[5] This is very important in the context of Quantum Gravity, where without a fixed background metric a restriction like "Euclidean invariance" will be too strong to ask for.

[6] From the OS data $(\mathcal{H}, \hat{H}, \Omega)$ it is straightforward to build a state, by simply defining it as $\omega(a) := \langle \Omega, \hat{a}\Omega \rangle_{\mathcal{H}}$.

[7] It must, however, be noted that it is not automatically granted that μ, as defined by this OS construction, is indeed a measure, i.e. a positive map such that $\mu(a) \geq 0 \;\forall a \geq 0$. This is the case for the free field, as we will learn later. However, in general more work is needed for this, see e.g. [173–176].

4. The Hamiltonian is defined as the self-adjoint operator that is the generator of the time-translations automorphism on $\mathcal{A} \supset \mathcal{E}$.
5. Find a (complete) set of observables (commuting with the constraints, if present). They represent the physical experiments whose outcomes our quantum theory can predict

II.A Mathematical Background

In this chapter we give an introduction to functional analysis and compile the basic notions from representations theory. We follow the textbooks [177–188], which also covers further details.

II.A.1 Functional Analysis

The proofs in the following subsection are partly taken from [177] and [178].

Definition II.A.1 (Cauchy sequence, Hilbert space)**.** *A* Pre-Hilbert space $\mathcal{H}'$ *is a complex vector space with a form*

$$\begin{aligned} \langle\, .\,,\,.\,\rangle : \mathcal{H}' \times \mathcal{H}' &\to \mathbb{C} \\ (\psi, \psi') &\mapsto \langle \psi, \psi' \rangle \end{aligned} \tag{II.9}$$

called scalar product *obeying the following properties*

1. *Symmetry: for all* $\psi,\ \psi' \in \mathcal{H}'$
$$\overline{\langle \psi, \psi' \rangle} = \langle \psi', \psi \rangle \tag{II.10}$$
2. *Sesqui-linearity: for all* $\psi,\ \psi_1,\ \psi_2 \in \mathcal{H}'$ *and* $z_1,\ z_2 \in \mathbb{C}$
$$\langle \psi, z_1\psi_1 + z_2\psi_2 \rangle = z_1\langle \psi, \psi_1 \rangle + z_2\langle \psi, \psi_2 \rangle \tag{II.11}$$
3. *Positive definiteness: for all* $\psi \in \mathcal{H}'$*:* $\langle \psi, \psi \rangle \geq 0$ *and* $\langle \psi, \psi \rangle = 0 \Leftrightarrow \psi = 0$.

Let $||\psi|| := \sqrt{\langle \psi, \psi \rangle}$*, called the norm of* $\mathcal{H}$*. We adopt the following notations*

- *A sequence* $(\psi_n)_{n\in\mathbb{N}}$ *with* $\psi_n \in \mathcal{H}'\ \forall n$ *is called* Cauchy sequence $\Leftrightarrow \forall \epsilon > 0$ *there exists* $N(\epsilon) \in \mathbb{N}$ *with* $||\psi_n - \psi_m|| < \epsilon$ *for all* $m, n > N(\epsilon)$.
- *A sequence is called* convergent *to* $\psi \in \mathcal{H}' \Leftrightarrow \forall \epsilon > 0$ *there exists* $N(\epsilon) \in \mathbb{N}$ *with* $||\psi - \psi_n|| < \epsilon$ *for all* $n > N(\epsilon)$.
- *A subspace* $U \subset \mathcal{H}'$ *is called* dense *in* $\mathcal{H}' \Leftrightarrow \forall \epsilon > 0,\ \psi \in \mathcal{H}'$ *there exists* $\psi' \in U$ *such that* $||\psi - \psi'|| < \epsilon$
- *A subspace* $U \subset \mathcal{H}'$ *is* closed $\Leftrightarrow$ *If* $\psi_n \in U$ *and* $(\psi_n)_{n\in\mathbb{N}}$ *convergent to* $\psi \in \mathcal{H}'$ *then* $\psi \in U$

Iff every Cauchy sequence of elements in a Pre-Hilbert space converges, it is called a Hilbert space*.*

Hence any element of $\mathcal{H}'$ can be approximated with arbitrary precision by elements of a dense subspace U.

Lemma II.A.1 (Cauchy-Schwarz inequality)**.** *Let* $\mathcal{H}'$ *be a Pre-Hilbert space. It holds for all* $\psi, \psi' \in \mathcal{H}'$*:*

$$|\langle \psi, \psi' \rangle| \leq ||\psi|| \cdot ||\psi'|| \tag{II.12}$$

and the equality is only true iff $\psi = \lambda\psi',\ \lambda \in \mathbb{C}$.

Proof. Since (II.12) is trivial for $\psi' = 0$ we assume in the following $\psi' \neq 0$ and define $\lambda = \langle \psi, \psi' \rangle / ||\psi'||^2$:

$$\begin{aligned} 0 \leq ||\psi - \lambda\psi'||^2 &= \langle \psi, \psi \rangle - \langle \lambda\psi', \psi \rangle - \langle \psi, \lambda\psi' \rangle + \langle \lambda\psi', \lambda\psi' \rangle = \\ &= ||\psi||^2 - \lambda\overline{\langle \psi, \psi' \rangle} - \overline{\lambda}\langle \psi, \psi' \rangle + |\lambda|^2||\psi'||^2 = ||\psi|| - |\langle \psi, \psi' \rangle|^2/||\psi'||^2 \end{aligned} \tag{II.13}$$

If both sides are equal, i.e. $||\psi - \lambda\psi'|| = 0$ hence $\psi - \lambda\psi' = 0$ by positive definiteness of the scalar product. On the other hand, if $\psi = \lambda\psi'$ follows

$$|\langle \psi, \psi' \rangle| = |\langle \lambda\psi', \psi' \rangle| = |\lambda||\psi'||^2| = |\lambda| \cdot ||\psi'||^2 = ||\lambda\psi'|| \cdot ||\psi'|| = ||\psi|| \cdot ||\psi'|| \tag{II.14}$$

which is the statement. □

Definition II.A.2 (Orthonormal basis). *Let $\mathcal{H}$ be a Hilbert space. A system $(e_I)_{I\in\mathcal{I}}$ of elements $e_I \in \mathcal{H}$ with some index set $\mathcal{I}$ is called an* orthonormal basis *if its finite linear combinations are dense in $\mathcal{H}$ and $\forall I, J \in \mathcal{I}$ holds $\langle e_I, e_J\rangle = \delta_{IJ}$.*[8]
We call a Hilbert space separable *if there exists an orthonormal basis with at most countable infinite $\mathcal{I}$.*

Lemma II.A.2 (Riesz-Lemma). *Let $l : \mathcal{H} \to \mathbb{C}$ be a bounded linear form. Then, there exists a unique $\xi_l \in \mathcal{H}$ such that $\forall\psi \in \mathcal{H}$*

$$l(\psi) = \langle \xi_l, \psi\rangle \tag{II.15}$$

Proof. If $l \equiv 0$ then $\xi_l = 0$. Let $l \neq 0$, then exists $l(\psi') = 1$ since e.g. $\psi' = \psi/l(\psi)$. So we call:

$$C_l = \{\psi \in \mathcal{H} \ : \ l(\psi) = 1\} \tag{II.16}$$

which is closed (pre-image of a single point) and convex, since

$$l(\frac{\psi+\psi'}{2}) = \frac{1}{2}l(\psi) + \frac{1}{2}l(\psi') = 1 \tag{II.17}$$

As l was bounded there exists a (due to convexity and (II.12)) unique $\tilde{\psi} \in C_l$, such that $||\tilde{\psi}|| = \inf_{\psi\in C_l} ||\psi||$.

$$C_l = \{\tilde{\psi} + \psi : \ \psi \in \mathcal{H}, \ l(\psi) = 0\} = \{\tilde{\psi} + \psi : \ \psi \in \mathcal{N}\} \tag{II.18}$$

where $\mathcal{N} = \{\psi \in \mathcal{H} : \ l(\psi) = 0\}$ is the null space of l. It follows that for all $\psi \in \mathcal{N}$ we have $\langle\psi, \tilde{\psi}\rangle = 0$ since

$$||\tilde{\psi} + t\psi||^2 = ||\tilde{\psi}||^2 + t\langle\psi, \tilde{\psi}\rangle + t\langle\tilde{\psi}, \psi\rangle + t^2||\psi||^2 \tag{II.19}$$

$\forall t$ due to convexity. However, by definition it must be smaller than $||\tilde{\psi}||$, hence $\langle\psi, \tilde{\psi}\rangle = 0$.
If $l(\psi') = 0 \Rightarrow \psi' \in \mathcal{N}$. On the other hand, if $l(\psi') = s$ then $l(\psi'/s) = 1 \Rightarrow \psi'/s \in C_l$. Thus, each $\psi' \in \mathcal{H}$ can be written as $\psi' = s\tilde{\psi} + \psi, \ \psi \in \mathcal{N}, \ s \in \mathbb{C}$. This yields

$$l(\psi') = l(s\tilde{\psi} + \psi) = sl(\tilde{\psi}) + l(\psi) = s \tag{II.20}$$

So, we conclude that each $\psi' \in \mathcal{H}$ can be uniquely written as $\psi' = l(\psi')\tilde{\psi} + \psi, \ l(\psi) = 0$ and hence:

$$\langle\psi', \tilde{\psi}\rangle = l(\psi')\langle\tilde{\psi}, \tilde{\psi}\rangle \ \Rightarrow \ l(\psi') = \langle\psi', \tilde{\psi}/||\tilde{\psi}||\rangle =: \langle\psi', \xi_l\rangle \tag{II.21}$$

□

Theorem II.A.1 (Bounded Operators). *Given two Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$ (with corresponding norms $||.||_1, \ ||.||_2$) we denote as operator any linear transformation $T : \mathcal{H}_1 \to \mathcal{H}_2$, i.e.*

$$T(z_1\psi + z_2\psi') = z_1T\psi + z_2T\psi', \qquad \forall z_1, z_2 \in \mathbb{C}, \forall\psi, \psi' \in \mathcal{H} \tag{II.22}$$

Then, the following statements are equivalent:

1. *T is* bounded *$\Leftrightarrow$ there exists $k \geq 0$ with $||T\psi||_2 \leq k||\psi||_1 \ \forall\psi \in \mathcal{H}$*
2. *T is* continuous *for all $\psi \in \mathcal{H} \Leftrightarrow \forall\epsilon > 0$ there exists $\delta(\epsilon) > 0$ with $||T\psi - T\psi'||_2 < \epsilon$, $\forall\psi' \in \mathcal{H}$ such that $||\psi - \psi'||_1 < \delta(\epsilon)$*
3. *T is continuous in $0 \in \mathcal{H}$*

Proof. 1. $\to$ 2. Since $\psi_n \to \psi$ in $\mathcal{H}$ is equivalent to $\lim_{n\to\infty} ||\psi_n - \psi||_1 = 0$, we deduce that

$$||T\psi_n - T\psi||_2 = ||T(\psi_n - \psi)||_2 \leq k||\psi_n - \psi||_1 \underset{n\to\infty}{\longrightarrow} 0 \tag{II.23}$$

2. $\to$ 3. is trivial. And for 3. $\to$ 1. we assume there is no k such that 1. is true, in other words $\forall n \in \mathbb{N}$ there exists $\psi_n \in \mathcal{H}$ such that $||T\psi_n||_2 > n||\psi_n||_1$. Let $\psi'_n = \psi_n/(n||\psi_n||_1)$ hence $||\psi'_n||_1 = 1/n \to 0$. Then

$$||T\psi'_n||_2 = \frac{||T\psi_n||_2}{n||\psi_n||_1} > 1 \tag{II.24}$$

implying that $T\psi'_n$ is not converging to $0 = T(0)$, hence not continuous in $0 \in \mathcal{H}$. □

In the following we denote the space of all linear operators from $\mathcal{H}_1$ to $\mathcal{H}_2$ as $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ and the space of all bounded operators as $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ and respectively $\mathcal{L}(\mathcal{H})$, $\mathcal{B}(\mathcal{H})$ if $\mathcal{H} = \mathcal{H}_1 = \mathcal{H}_2$. In general, an operator T might only be defined on a subset called $D(T) \subset \mathcal{H}$.

[8] The existence of an ONB is guaranteed for any Hilbert space by the axiom of choice [189] and the *Gram-Schmidt process* [185].

Theorem II.A.2 (Continuous linear extension theorem)**.** *Let $T \in \mathcal{B}(\mathcal{H}', \mathcal{H})$, with $\mathcal{H}$ being a Hilbert space and $\mathcal{H}'$ a Pre-Hilbert space. Then there exists a unique extension of T, called $\tilde{T}$ from the completion $\tilde{\mathcal{H}}$ of $\mathcal{H}'$.*
Also, for the norm of T *holds:* $||T||' = ||T||^{\sim}$, *where* $||T||' = \sup_{\psi \notin 0} \frac{||T\psi||}{||\psi||'}$.

Proof. First we show uniqueness: be $\tilde{T} : \tilde{\mathcal{H}} \to \mathcal{H}$ such an extension, then for any $\psi \in \tilde{\mathcal{H}}$ and $\psi_n \in \mathcal{H}'$ such that $\psi_n \to \psi$ we get due to continuity of $\tilde{T}$:

$$\tilde{T}\psi = \lim_n \tilde{T}\psi_n = \lim_n T\psi_n \tag{II.25}$$

in other words, $\tilde{T}$ is uniquely determined by T.
Regarding existence , choose $\psi \in \tilde{\mathcal{H}}$ and $\psi_n \in \mathcal{H}'$ a Cauchy sequence with $\psi_n \to \psi$. Then, $(T\psi_n)_{n\in\mathbb{N}}$ is also a Cauchy sequence, due to $||T\psi_n - T\psi_m||' \leq ||T|| \cdot ||\psi_n - \psi_m||)$. With $\mathcal{H}$ being a Hilbert space, $(T\psi_N)$ is convergent. We choose for each $\psi \in \tilde{\mathcal{H}}$ a sequence $\psi_n \in \mathcal{H}'$ such that $\psi_n \to \psi$

$$\tilde{T}\psi := \lim_n T\psi_n \tag{II.26}$$

(which is independent on the choice of the particular ψ_n). That this extension is also linear is seen by considering two sequences $\psi_n \to \psi$, $\psi'_n \to \psi$ and

$$\tilde{T}(a\psi + b\psi') = \lim_n T(a\psi_n + b\psi'_n) = a \lim_n T\psi_n + b \lim_n T\psi'_n = a\tilde{T}\psi + b\tilde{T}\psi' \tag{II.27}$$

Lastly, we show that $||\tilde{T}|| = ||T||$, i.e. $\tilde{T}$ is continuous: Obviously $||\tilde{T}|| \geq ||T||$. But $\psi \in \tilde{\mathcal{H}}$ and $\psi_n \to \psi$ give

$$||\tilde{T}\psi|| = \lim_n ||T\psi_n|| \leq \lim_n ||T|| \cdot ||\psi_n|| = ||T|| \cdot ||\psi|| \tag{II.28}$$

thus $||\tilde{T}|| \leq ||T||$. □

Lemma II.A.3. *Let $T \in \mathcal{L}(\mathcal{H})$ be densely defined, i.e. $D(T) \subset \mathcal{H}$. Let*

$$D(T^\dagger) := \{\psi \in \mathcal{H}, \sup_{0 \neq \psi \in D(T)} \frac{|\langle \psi, T\psi' \rangle|}{||\psi'||} < \infty\} \tag{II.29}$$

Then, there exists a linear operator $T^\dagger$ uniquely defined by

$$\langle T^\dagger \psi, \psi' \rangle = \langle \psi, T\psi' \rangle, \qquad \forall \psi \in D(T^\dagger),\ \psi' \in D(T) \tag{II.30}$$

Proof. Consider the following linear form for each $\psi \in D(T^\dagger)$

$$L_\psi(\psi') = \langle \psi, T\psi' \rangle \tag{II.31}$$

on $D(T)$. Since $\psi \in D(T^\dagger)$, it follows that $L_\psi(\ .\ )$ is a bounded linear transformation, mapping from $(D(T), ||.||)$ to the Cauchy-complete space $(\mathbb{C}, ||.||_{\mathbb{C}})$ with $||z||_{\mathbb{C}} = |z|$. Thus, we can invoke the continuous linear extension theorem II.A.2 in order to promote L_ψ uniquely to $\tilde{L}_\psi$ on $\overline{D(T)} = \mathcal{H}$ with respect to $||.||$ on $\mathcal{H}$. And with the Riesz-Lemma II.A.2 we deduce the existence of a unique element $\xi_{\tilde{L}_\psi} \in \mathcal{H}$ such that $\forall \psi' \in \mathcal{H}$:

$$\langle \xi_{\tilde{L}_\psi}, \psi' \rangle = \tilde{L}_\psi(\psi') \tag{II.32}$$

Thus, we can define an operator $T^\dagger$ on $D(T^\dagger)$ as $T^\dagger\psi := \xi_{\tilde{L}_\psi}$.
Defined in such way $T^\dagger$ is indeed linear as $\forall \psi_1, \psi_2 \in D(T^\dagger),\ \psi' \in D(T)$:

$$\begin{aligned} \langle T^\dagger(z_1\psi_1 + z_2\psi_2), \psi' \rangle &= \langle z_1\psi_1 + z_2\psi_2, T\psi' \rangle = \bar{z}_1 \langle \psi_1, T\psi' \rangle + \bar{z}_2 \langle \psi_2, T\psi' \rangle = \\ &= \bar{z}_1 \langle T^\dagger\psi_1, \psi' \rangle + \bar{z}_2 \langle T^\dagger\psi_2, \psi' \rangle = \langle z_1 T^\dagger\psi_1, \psi' \rangle + \langle z_2 T^\dagger\psi_2, \psi' \rangle = \langle (z_1 T^\dagger\psi_1 + z_2 T^\dagger\psi_2), \psi' \rangle \end{aligned} \tag{II.33}$$

□

Definition II.A.3 (Unitary and self-adjoint operators)**.** *Let $T \in \mathcal{L}(\mathcal{H})$. It is called* unitary *if $D(U) = \mathcal{H}$, $U\mathcal{H} = \mathcal{H}$ and $\forall \psi \in \mathcal{H}$ it fulfils the* isometry *condition*

$$||U\psi|| = ||\psi|| \tag{II.34}$$

We will call T self-adjoint[9] *if it is densely defined on $\mathcal{H}$, $D(T) = D(T^\dagger)$ and*

$$T\Psi = T^\dagger\Psi, \qquad \forall \Psi \in D(T) \tag{II.35}$$

[9] In physics these operators play a special role as one can easily see that they have real spectrum, i.e. $\sigma(T) \subset \mathbb{R}$.

II.A.2 Measures on Lie groups and Lie algebras

We adapt a didactic approach to Lie groups and Lie algebras which is due to [179] and supplement it with proofs from [180].

Definition II.A.4 (Lie groups, Lie algebras)**.** *A* Lie group *is a smooth manifold G that also forms a group via a smooth group product $G \times G \to G$ and a smooth inverse map $g \to g^{-1}$.*
A complex Lie algebra $\mathfrak{g}$ *is a complex vector space together with a bilinear, antisymmetric* Lie bracket

$$\begin{aligned} [\cdot,\cdot]: \ & \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g} \\ & a \times b \mapsto [a,b] \end{aligned} \tag{II.36}$$

which obeys the Jacobi identity $\forall a,b,c \in \mathfrak{g}$:

$$[a,[b,c]] + [b,[c,a]] + [c,[a,b]] = 0 \ . \tag{II.37}$$

A unital $*$-Algebra $\mathcal{A}$ *is an algebra with unit element $\mathbb{1}_{\mathcal{A}} \in \mathcal{A}$ with respect to multiplication and* involution*, i.e. an antilinear map such that $a,b \in \mathcal{A} \ \Rightarrow \ (ab)^* = b^*a^*$, $(a^*)^* = a$ and $(za)^* = \bar{z}a^*$ for $z \in \mathbb{C}$. We can endow it with a Lie algebra structure by defining an antisymmetric bracket obeying (II.37).*

One should note that with any Lie group G one can associate a Lie algebra $\mathfrak{g}$ by considering the space of all tangent vectors at the identity of G. For all $h \in G$, the left translation diffeomorphism $L_h : G \to G$ is defined as

$$L_h g := gh, \qquad \forall g,h \in G \tag{II.38}$$

We say that a tangent vector field[10] $v \in TG$ is *left-invariant* iff $(L_h)_* v \mid_g = v \mid_{ga}$, where the push-forward is defined as $\phi_*(v)(.) := v(\phi(.))$ for all $\phi \in \mathsf{Diff}(G)$. The space of all left-invariant tangent vectors at the identity is the Lie algebra $\mathfrak{g} = \mathfrak{g}(G)$, equipped the commutator of vector fields as Lie bracket.
We construct an isomorphism from $\mathfrak{g}$ to G called the *exponential map*: for any left–invariant vector field v we associate the integral curves on G of v passing through id_G, i.e. the associated one parameter subgroup $g(t)$. Then we define $\forall v \in \mathfrak{g}$: $\exp(tv) := g(t)$.[11]

Definition II.A.5 (Measure, Lebesgue integral)**.** *Let Γ be the σ-algebra of a Lie group, i.e. a collection of all subsets including G, the empty set, for each $U \in \Gamma$ its complement and being closed under countable unions. The triple (G,Γ,μ) is called a* measure space*, where the* measure $\mu : \ \Gamma \to \mathbb{R}$ *is a map obeying:*

1. *Non-negativity: $\forall E \in \Gamma \ : \mu(E) \geq 0$.*
2. *Null empty set: for the empty set $E_\varnothing = \{\varnothing\}$ is $\mu(E_\varnothing) = 0$.*
3. *σ-additivity: for all countable collections $\{E_i\}_{i=1}^\infty$ of pairwise disjoint sets:*

$$\mu(\bigcup_k E_k) = \sum_k \mu(E_k) \ . \tag{II.39}$$

For any $E \in \Gamma$ the characteristic function $\chi_E : G \to \mathbb{C}$ *is such that $\chi_E(x) = 1$ if $x \in E$ and $\chi_E(x) = 0$ otherwise. A function $s : G \to \mathbb{C}$ of the form $s = \sum_{k=1}^N z_k \chi_{E_k}$ with $N < \infty$, $z_k \in \mathbb{C}$ is called* simple*.*
Given a measure space (G,Γ,μ) the Lebesgue integral *of a Borel measurable function $f \in C^\infty(G)$ is defined by (with s being simple)*

$$\mu(f) := \int_G d\mu(g) \ f(g) := \sup_{0 \leq s \leq f} \sum_{k=1}^{N(s)} z_k(s) \mu(E_k(s)) \ . \tag{II.40}$$

The supremum in (II.40) is understood by decomposing the real and the imaginary part of a complex valued function f in positive and negative contributions f_+, f_-. For the positive part we consider sequences s_n of simple functions smaller than f_+ pointwise almost everywhere with respect to μ and take the supremum of all such sequences. Then we continue analogously with $(-f_-)$.

[10] I.e. a linear map, $v : C^\infty(G) \to C^\infty(G)$. See the later section IV.A *Differential Riemannian Geometry* for more details.
[11] While largely unintuitive in this abstract formalism, once we introduce representations, the name exp becomes clear: the matrix exponential of an operator $t\pi(v)$ defines a group representation $\Pi(g(t))$.

Definition II.A.6 (Haar measure). *Given a finite-dimensional Lie group G and let for each $h \in G$ be λ_h/ρ_h the operators of left/right translations, i.e. $\lambda_h f(g) := f(hg)$ and $\rho_h f(g) := f(gh)$ for any smooth function $f : G \to \mathbb{R}$.*
A left/right-invariant Haar measure μ^l/μ^r *on G satisfies $\forall h \in G$:*

$$\mu^l(f) = \mu^l(\lambda_h^* f), \qquad \mu^r(f) = \mu^r(\rho_h^* f) \tag{II.41}$$

Theorem II.A.3. *If G is a finite-dim. (not necessarily compact) semi-simple Lie group then both μ^l and μ^r exist and are unique up to a constant. If G is compact then in fact $\mu_G := \mu^l = \mu^r$ if we normalise, i.e. demand that $\mu(1) = 1$. Its explicit form is given by: ($Z \in \mathbb{C}$, $n = \dim(G)$)*

$$d\mu(g) := \frac{1}{Z}\sqrt{\det(k(t))}d^n t|_{g=\exp(t)} \ . \tag{II.42}$$

Proof. If G is not connected, let G_0 be the component containing the identity id_G of G. Then all other components are of the form $G_n = g_n \cdot G_o$ with $g_n \in G$. Suppose μ_0^l is left-invariant on G_0, then

$$\mu^l(f) := \sum_n \mu_0^l(\lambda_{g_n}^* f) \tag{II.43}$$

is left-invariant on all of G and in fact independent of the choice of $g_n \in G_n$. Conversely if μ^l is left-invariant on all of $G = \bigcup_n G_n$, then

$$\mu^l(f) = \sum_n \mu^l|_{G_0}(\lambda_{g_n}^* f) \tag{II.44}$$

Hence μ^l is determined once we know it on G_0 and we can restrict our attention to connected Lie groups G. We will first show the uniqueness and afterwards the existence by explicit construction. So let $f \in C(G)$ be non-negative and not identically zero and let f' be arbitrary. Then for two left-invariant measures μ, μ'

$$h(g, g') := \frac{f(g'g)f'(g)}{\int_G d\mu'(t)f(tg)} \tag{II.45}$$

is well defined on $G \times G$ and continuous. Then we can use a generalisation of Fubini's theorem (which allows us to interchange integrations) and use the left-invariance of μ and μ':

$$\begin{aligned}\int_G d\mu(g)\int_G d\mu'(g')h(g,g') &= \int_G d\mu'(g')\int_G d\mu(g)h(g,g') = \int_G d\mu'(g')\int_G d\mu(g)h(g'^{-1}g,g') = \\ &= \int_G d\mu(g)\int_G d\mu'(g')h(g'^{-1}g,g') = \int_G d\mu(g)\int_G d\mu'(g')h(g'^{-1},gg')\end{aligned} \tag{II.46}$$

And thus (inserting a one in the first step)

$$\begin{aligned}\int_G d\mu(g)f'(g) &= \int_G d\mu(g)f'(g)\frac{\int_G d\mu'(g')f(g'g)}{\int_G d\mu'(t)f(tg)} = \int_G d\mu(g)\int_G d\mu'(g')\frac{f'(g)f(g'g)}{\int_G d\mu'(t)f(tg)} = \\ &= \int_G d\mu(g)\int_G d\mu'(g')h(g,g') = \int_G d\mu(g)\int_G d\mu'(g')h(g'^{-1},gg') = \\ &= \int_G d\mu(g)\int_G d\mu'(g')\frac{f'(g'^{-1})f(g)}{\int_G d\mu'(t)f(tg'^{-1})} = \int_G d\mu(g)f(g)\cdot\left(\int_G d\mu'(g')\frac{f'(g'^{-1})}{\int_G d\mu'(t)f(tg'^{-1})}\right)\end{aligned} \tag{II.47}$$

Thus, there is a constant c independent of μ such that

$$\frac{\int_G f'(g)d\mu(g)}{\int_G f(g)d\mu(g)} = c \tag{II.48}$$

Since c does not depend on μ, it is the same for μ' and hence follows $\forall f'$

$$\int_G f'(g)d\mu'(g) = \left(\frac{\int_G f(g)d\mu'(g)}{\int_G f(g)d\mu(g)}\right)\int_G f'(g)d\mu(g) =: a\int_G f'(g)d\mu(g) \tag{II.49}$$

Thus, the linear functionals $\mu(f')$, $\mu'(f')$ for $f' \in C(G)$ are the same up to a constant $\mu'(f') = a\mu(f')$ and it follows: $\mu' = a\mu =: \mu^l$.

Moreover, this unique left-inv. measure μ^l coincides with the right-inv. measure μ^r in case of compact G, as upon considering for an arbitrary but fixed $g_0 \in G$

$$\mu(f) := \int_G d\mu^r(h) f(g_0 h g_0^{-1}) \tag{II.50}$$

it follows $\mu(\rho^*_{g'} f) = \mu(f)$ due to right-inv. of μ^r and $\mu = \kappa(g_0)\mu^r$ by uniqueness. Using compactness, we may normalise μ^r

$$\kappa(g_0) = \kappa(g_0)\mu^r(G) = \mu(G) = \int_G d\mu^r(g) = 1 \tag{II.51}$$

which is independent of g_0. And thus $\forall g_0 \in G$:

$$\mu(f) = \int_G d\mu^r(g) f(g) = \int_G d\mu^r(g) f(g_0 g {g_0}^{-1}) = \int_G d\mu^r(g) f(g_0 g) \tag{II.52}$$

So, μ is also left-invariant, i.e. $\mu = \mu^l = \mu^r$.
Lastly, for its existence, we follow [50] and consider the bijective exponential map $\exp : \mathfrak{g} \to G$. Since $\exp(s)\exp(t) \in G$ there exists a $c \in G$ such that $\exp(c) = \exp(s)\exp(t)$ which is unique due to the exponential map being bijective, in other words $c(s,t)$ is a composition function such that

$$\exp(s)\exp(t) =: \exp(c(s,t)) \tag{II.53}$$

Now $\partial_{t^J} e^t = (e^s)^{-1}(\partial_{r^M} e^r)\mid_{r=c(s,t)} \partial_{t_J} c^M(s,t)$ and it follows:

$$\begin{aligned} k_{JK}(t) &= (\partial_{t^J} c^M)(\partial_{t^K} c^N) tr\left((e^s)^{-1}(\partial_{r^M} e^r)\mid_{r=c(s,t)} (\partial_{r^N} e^r)\mid_{r=c(s,t)} e^s\right) \\ &= (\partial_{t^J} c^M)(\partial_{t^K} c^N) k_{MN}(c(s,t)) \end{aligned} \tag{II.54}$$

and thus for the measure: $(\det(c^2 q) = \det(c^2)\det(q))$

$$\begin{aligned} \mu(\lambda_s^* f) &= \int_G d^n t \sqrt{\det(k(t))} f(\exp c(s,t)) = \int_G d^n r \frac{\sqrt{\det(k(t))}}{|\det(\partial c(s,t)/\partial t)|_{c(s,t)}} f(e^r) \\ &= \int_G d^n r f(e^r) \sqrt{\det(k(r))} = \mu(f) \end{aligned} \tag{II.55}$$

A similar calculation for right translation and inversion gives the statement. □

II.A.3 Representation Theory

In the following we will carefully distinguish between representations of groups and of $*$-algebras. This subsection follows closely [50].

Definition II.A.7 (Representation of a group / $*$-algebra)**.** *Let G be a Lie group. A* group representation *$(\Pi, \mathcal{H})$ of G consists of a map*

$$\Pi : \; G \to \mathcal{B}(\mathcal{H}) \tag{II.56}$$

$$g \mapsto \Pi(g) \tag{II.57}$$

onto the bounded operators on a Hilbert space $\mathcal{H}$, which are defined on a dense, invariant subspace D, i.e. $\Pi(g)D \subset D \subset \mathcal{H} \;\; \forall g \in G$ and obey the following properties

1. $\Pi(\mathrm{id}_G) = \mathrm{id}_{\mathcal{H}} =: \mathbb{1}$
2. $\Pi(gh) = \Pi(g)\Pi(h)$
3. $\Pi(g^{-1}) = \Pi(g)^{-1}$

For a unital $*$-algebra with Lie-algebra structure, $\mathcal{A}$, a representation $(\pi, \mathcal{H})$ with $\pi : \mathcal{A} \to \mathcal{L}(\mathcal{H})$ shall fulfil: $(a, b, \in \mathcal{A},\; z_1, z_2 \in \mathbb{C})$

1. $\pi(\mathbb{1}_{\mathcal{A}}) = \mathrm{id}_{\mathcal{H}} =: \mathbb{1}$

2. $\pi(ab) = \pi(a)\pi(b)$

3. $\pi(a^*) = \pi(a)^\dagger$

4. $\pi(z_1 a + z_2 b) = z_1\pi(a) + z_2\pi(b)$

We will adopt the following notations likewise for group and algebra representations:

Definition II.A.8. *A representation of* $(\pi, \mathcal{H})$ *is called*

1. cyclic *with* cyclic vector *or* vacuum $\Omega \Leftrightarrow$ *there exists* Ω *with* $\pi(\mathcal{A})\Omega := \{\pi(a)\Omega, a \in \mathcal{A}\}$ *dense in* $\mathcal{H}$.

2. irreducible $\Leftrightarrow$ *every vector* $0 \neq \psi \in D \subset \mathcal{H}$ *is cyclic* $\Leftrightarrow \nexists$ *invariant subspaces other than* $\mathcal{H}$ *and* $\{0\}$

3. faithful *iff it is injective*

4. finite dimensional $\Leftrightarrow \dim(\mathcal{H}) < \infty$

5. unitary $\Leftrightarrow \pi(a)^\dagger = \pi(a)^{-1}$, *i.e. all operators are unitary*

6. completely reducible *iff it decomposes into a direct sum of irreducible representations* $\pi^{(j)}$ *on the spaces* $\mathcal{H}^{(j)}$, *that is*

$$\pi = \oplus_j \pi^{(j)}, \qquad \mathcal{H} = \oplus_j \mathcal{H}^{(j)} \tag{II.58}$$

7. unitary equivalent *with another representation* $(\pi', \mathcal{H}') \Leftrightarrow$ *there exists a (unitary) isomorphism* $U : \mathcal{H} \to \mathcal{H}'$ *such that* $\forall a \in \mathcal{A}:\ U\pi(a)U^\dagger = \pi'(a)$

And similar for $(\Pi, \mathcal{H})$.

Theorem II.A.4. *Let* $\mathcal{A}$ *be a unital *-algebra with Lie-algebra structure. Then every representation* $(\pi, \mathcal{H})$ *is a direct sum of cyclic representations.*

Proof. This is taken from [181]. First note that existence of a unit element guarantees automatically non-degeneracy, i.e. $\pi(a)\psi = 0\ \forall a \in \mathcal{A}$ implies $\psi = 0$. Then, we consider the maximal set $(\mathcal{H}^{(j)})_{j\in\mathcal{J}}$ of all pairwise orthogonal, closed and invariant subspaces on which π is cyclic.
Let $K := \overline{\oplus_j \mathcal{H}^{(j)}}$, i.e. the closure of the direct sum of Hilbert spaces. With $\mathcal{H}^{(j)}$ being invariant and $\pi(a)$ continuous $\forall a \in \mathcal{A}$, follows that K is invariant, too. Hence also $K^\perp$, the orthogonal complement of K in $\mathcal{H}$, since for $\psi \in K^\perp$ and $\psi' \in K$ follows for all $a \in \mathcal{A}$:

$$\langle \pi(a)\psi, \psi' \rangle = \langle \psi, \pi(a)^\dagger \psi' \rangle = 0 \tag{II.59}$$

because $\pi(a)^\dagger \psi \in \pi(\mathcal{A})K \subseteq K$. The statement would follow if $K^\perp = 0$. Hence we assume that $K^\perp \neq 0$. Then exists $0 \neq \psi \in K^\perp$ and we define

$$C = \overline{\text{span}\ \pi(\mathcal{A})\psi} \tag{II.60}$$

which is also a closed, invariant subspace. We write $\psi = \psi_0 + \psi'$ with $\psi' \in C$ and $\psi_0 \perp C$. With $C^\perp$ being invariant, follows:

$$C \ni \pi(a)\psi = \pi(a)\psi_0 + \pi(a)\psi' \tag{II.61}$$

But since $\pi(a)\psi_0 \in C^\perp$, it must vanish for all $a \in \mathcal{A}$. But $(\pi, \mathcal{H})$ is non degenerate, thus $\psi_0 = 0$. This means $\psi \in C$ and hence the representation is cyclic on C. This implies a contradiction to the maximality of $(\mathcal{H}^{(j)})_{j\in\mathcal{J}}$. □

One can quickly see that the same holds true for Lie groups which carry an involution and non-degenerate representations thereof. Thus, we can restrict our attention to the construction of cyclic representations and, moreover, to unitary ones as:

Lemma II.A.4. *Let* G *be a compact, finite-dim Lie group and* $(\Pi, \mathcal{H})$ *a continuous finite-dim representation of* G. *Then we may replace the scalar product on* $\mathcal{H}$ *by one with respect to which* Π *is unitary.*

Proof. We denote with $\langle .,. \rangle'$ the old scalar product on $\mathcal{H}$ and define a new scalar product by

$$\langle \psi, \psi' \rangle := \int_G d\mu_G(g) \langle \Pi(g)\psi, \Pi(g)\psi' \rangle' \tag{II.62}$$

which is due to Π being continuous and G compact:

$$|\langle \psi, \psi' \rangle| \leq (\int_G \mu_G(g)\ 1)\ \sup_{g\in G} |\langle \Pi(g)\psi, \Pi(g)\psi' \rangle'| < \infty \tag{II.63}$$

With this we can easily check $\forall g' \in G$: $(\tilde{g} := gg')$

$$\begin{aligned}\langle \psi, \Pi(g')\psi' \rangle &= \int_G d\mu_G(g) \langle \Pi(g)\psi, \Pi(g)\Pi(g')\psi' \rangle' = \int_G d\mu_G(\tilde{g}) \langle \Pi(\tilde{g})\Pi({g'}^{-1})\psi, \Pi(\tilde{g})\psi' \rangle' = \\ &= \langle \Pi({g'}^{-1})\psi, \psi' \rangle = \langle \Pi(g')^\dagger \psi, \psi' \rangle \end{aligned} \tag{II.64}$$

Giving the statement: $\Pi(g')^\dagger = \Pi({g'}^{-1}) = \Pi(g')^{-1}$. □

Lemma II.A.5 (Schur)**.** *Suppose $(\Pi_j, \mathcal{H}^j)$ $j = 1, 2$ are finite-dim irreducible representations of G and there exists an intertwiner: $A : \mathcal{H}^1 \to \mathcal{H}^2$ such that $\Pi_2(g)A = A\Pi_1(g)$ for all $g \in G$. Then:*
1. Either $A = 0$
2. Or A is invertible, unique up to a constant ($A = \kappa\mathbb{1}$) and we call $(\Pi_1, \mathcal{H}^1)$ and $(\Pi_2, \mathcal{H}^2)$ equivalent.

Proof. Let $V_1 = ker(A) \subset \mathcal{H}^1$, $V_2 = Im(A) \subset \mathcal{H}^2$. Let $\psi \in ker(A)$ then $A\Pi_1(g)\psi = \Pi_2(g)A\psi = 0 \Rightarrow$ V_1 is invariant. Let $\phi \in Im(A)$, then exists $\psi \in \mathcal{H}^1$ such that $\phi = A\psi$ and $\Pi_2(g)A\psi = A\Pi_1(g)\psi \Rightarrow V_2$ is invariant.
Now since Π_1 is Irrep $\Rightarrow$ either $V_1 = \mathcal{H}^1$ (i.e. $A = 0$) or $V_1 = \{0\}$ (i.e. A is injective). And since Π_2 is Irrep $\Rightarrow$ either $V_2 = \{0\}$ (i.e. $A = 0$) or $V_2 = \mathcal{H}_2$ (i.e. A is surjective).
Now let A be an intertwiners for case 2., then exists $\kappa \in \mathbb{C}$ such that $A - \kappa\mathbb{1}$ is singular. But since $A - \kappa\mathbb{1}$ is an intertwiner we are in case 1. and $A - \kappa\mathbb{1} = 0$. □

This Lemma (due to [190]) but found many application in representation theory. We will use it in the proof of the following theorem [191]

Theorem II.A.5 (Peter & Weyl)**.** *Let j be a labelling of the equivalence classes of finite-dim., irreducible, unitary representations $(\Pi^{(j)}, \mathcal{H}^{(j)})$ of compact G and define*

$$b_{jmn}(g) := \sqrt{d_j}\Pi^{(j)}_{mn}(g) \tag{II.65}$$

with $m, n \in \{1...d_j\}$ and $d_j = \dim(\mathcal{H}^{(j)})$.
Then the b_{jmn} form an orthonormal basis of the Hilbert space $\mathcal{H} = L_2(G, d\mu_G)$, where μ_G is the Haar measure on G, i.e. $\forall f, h \in \mathcal{H}$:

$$\langle f, h \rangle := \int_G d\mu_G(g)\ \overline{f(g)}h(g) \tag{II.66}$$

Proof. This taken from [50]. First, we show that

$$\langle b_{jmn}, b_{j'm'n'} \rangle = \delta_{jj'}\delta_{mm'}\delta_{nn'} \tag{II.67}$$

which we call $A^{jj'}_{nn'}(mm') := \langle b_{jmn}, b_{j'm'n'} \rangle$, i.e. a matrix with entries labelled by n, n' ($n = 1, ..., d_j$, $n' = 1, ..., d_{j'}$) with additional labels j, j', m, m'. First, we show that $A^{jj'}(m, m')$ is an intertwiner between $(\Pi^{(j')}, \mathcal{H}^{(j)})$ and $(\Pi^{(j)}, \mathcal{H}^{(j)})$:

$$\begin{aligned}[A^{jj'}(m, m')\Pi^{(j')}(g)]_{nn'} &= \sum_{\tilde{n}} A^{jj'}_{n\tilde{n}}(m, m')\Pi^{(j')}_{\tilde{n}n'}(g) = \\ &= \sqrt{d_j d_{j'}} \int_G d\mu_G(h)\ \overline{\Pi^{(j)}_{mn}(h)}\Pi^{(j')}_{m'n'}(hg) = [\Pi^{(j)}(g)A^{jj'}(m, m)]_{nn'}\end{aligned} \tag{II.68}$$

where we used unitarity: $\overline{\Pi^{(j)}_{\tilde{n}n}(g^{-1})} = \Pi^{(j)}_{n\tilde{n}}(g)$.
For non-vanishing A, by Schur, j and j' must be equivalent and then A is fixed up to a constant κ, i.e.:

$$A^{jj'}_{nn'}(m, m') = \delta_{jj'}A^{jj'}_{nn'}(m, m') = \delta_{jj}\delta_{nn'}\kappa^{jj'}(m, m') \tag{II.69}$$

To determine κ, we compute the trace

$$\sum_{n=n'} \delta_{jj'}\delta_{nn'}\kappa^{jj'}(m,m') = d_j\delta_{jj'}\kappa^{jj'}(m,m') = \sum_{n=n'} d_j \int_G d\mu_g(h)\overline{\Pi^{(j)}_{mn}(h)}\Pi^{(j)}_{m'n'}(h) = d_j\delta_{mm} \tag{II.70}$$

where we used unitarity, that $\Pi^{(j)}_{mm'}(\mathrm{id}_G) = \delta_{mm'}$ and that $\mu_G = 1$.
Now we want to prove that the span of the b_{jmn} is dense in $L_2(G, d\mu_G)$. Let $\mathfrak{B} \subset C(G)$ be the subalgebra of the abelian C^*-algebra of continuous functions on G generated by the b_{jmn}, so $\mathfrak{B}$ contains finite linear combinations and products of the b_{jmn}.
$b_{jmn}b_{j'm'n'}$ can be considered as matrix e' of $\Pi^{(j)} \otimes \Pi^{(j')}$ which is finite-dim, thus completely reducible to sums of the $\Pi^{(j)}$ again. In other words, $\mathfrak{B}$ is the finite linear span of the b_{jmn}. As one can see from the general theory of Hausdorff spaces $C(G)$ is dense in $L_2(G, d\mu_G)$. Now given $\psi \in L_2(G, d\mu_G)$, then there exists $f \in C(G)$ such that $||\psi - f||_{L_2} < \epsilon/2$ with $\epsilon > 0$. For this f, there exists $b \in \mathfrak{B}$ such that $||f - b||_\infty = \sup_{g\in G} |f(g) - b(g)| < \epsilon/2$. Then

$$||f - b||^2_{L_2} = \int_G d\mu_G(g)|(f - b)(g)|^2 \leq ||f - b||^2_\infty < (\epsilon/2)^2 \tag{II.71}$$

And finally

$$||\psi - b||_{L_2} \leq ||\psi - f||_{L_2} + ||f - b||_{L_2} < \epsilon \tag{II.72}$$

□

II.B Canonical vs Covariant Quantisation

We will review two of the many possible ways to quantise a system, which both yield the same unique result in case of a regular state in a finite dimensional system due to the *Stone-von Neumann theorem* [192–195]. Since a field theory carries infinitely many degrees of freedom the situation looks different and both cases will have to be discussed separately.

II.B.1 Canonical Quantisation

Given an action $S[\phi_I]$ of a system with some field degrees of freedom living on a manifold $\mathcal{M} \cong \sigma \times \mathbb{R}$ (with σ being a spatial submanifold), we will perform a Legendre transformation to obtain the corresponding Hamilton function $H(\phi_I, \pi_{\phi_I})$, defined on a classical phase space $\mathcal{F}$ with symplectic structure $\{\pi^J_\phi(y), \phi_I(x)\} = \delta^J_I\delta^{(3)}(x, y)$.
The structure of this subsubsection follows the programme of canonical quantisation, see e.g. [50].

Gel'fand-Naimark-Segal Construction

The first step towards defining a canonical quantum theory is the choice of a quantum $*$-algebra of observables.

Definition II.B.1 (Algebra of observable, states)**.** *Let $\mathcal{E}$ be a sub set of $C^\infty(\mathcal{F})$ such that it is*

1. *closed under complex conjugation, i.e. $\mathcal{E} = \overline{\mathcal{E}}$*
2. *closed with respect to the symplectic structure, i.e. $\{\mathcal{E}, \mathcal{E}\} \subseteq \mathcal{E}$*
3. *separating points, i.e. $f(\phi, \pi) = f(\phi', \pi')\ \forall f \in \mathcal{E} \Rightarrow (\phi, \pi) = (\phi', \pi')$*
4. *including the constant functions, i.e. $1 \in \mathcal{E}$*

We construct the free algebra *$\mathcal{A}'$, i.e. the non-commutative $*$-algebra of* books *and* words *from $\mathcal{E}$ where a word* w *is a formal multiplication of finitely many $f_k \in \mathcal{E}$ and a book* b *a formal linear combination of finitely many words*

$$\mathrm{b} = \mathrm{w}_1 + ... + \mathrm{w}_\mathrm{M}, \qquad \mathrm{w} = f_1 \cdot ... \cdot f_N, \quad f_k \in \mathcal{E} \tag{II.73}$$

The algebra of observables $\mathcal{A}$ *is now simply the quotient*

$$\mathcal{A} = \mathcal{A}'/J \tag{II.74}$$

with the two sided ideal, i.e. $\mathrm{b}J = J\mathrm{b}'$ *for all* $\mathrm{b}, \mathrm{b}' \in \mathcal{A}'$,

$$J = \{\mathrm{b}(f \cdot g - g \cdot f - i\hbar\{f,g\})\mathrm{b}',\ \mathrm{b}, \mathrm{b}' \in \mathcal{A}',\ f,g \in \mathcal{E}\} \tag{II.75}$$

for some $\hbar \in \mathbb{R}$.
A state *on* $\mathcal{A}$ *is a positive linear functional* $\omega : \mathcal{A} \to \mathbb{C}$ *such that*

$$\omega(z_1 a_1 + z_2 a_2) = z_1\omega(a_1) + z_2\omega(a_2), \qquad \omega(a^* a) \geq 0, \qquad \omega(\mathbb{1}_{\mathcal{A}}) = 1 \tag{II.76}$$

One can easily convince oneself that the equivalence class $[\mathrm{b}] = [\mathrm{b} + j,\ j \in J]$ is independent of the choice of representative and that the following relations hold:

$$[\mathrm{b}] + [\mathrm{b}'] = [\mathrm{b} + \mathrm{b}'], \qquad [\mathrm{b}] \cdot [\mathrm{b}'] = [\mathrm{b}\mathrm{b}'], \qquad [\mathrm{b}]^* = [\mathrm{b}^*] \tag{II.77}$$

Given an algebra of observables and a state thereon the *GNS construction* [169, 170] builds a corresponding representation thereof:

Theorem II.B.1 (Gel'fand, Naimark, Segal)**.** *Let* $\mathcal{A}$ *be a unital* $*$*-algebra and* ω *a state on* $\mathcal{A}$*. Then there exists (up to unitary equivalence) a unique correspondence between* ω *and a cyclic representation* $(\pi, \mathcal{H}, \Omega)$ *given by the* vacuum expectation value of $\pi(a)$*:*

$$\omega(a) = \langle \Omega, \pi(a)\Omega\rangle_{\mathcal{H}} \tag{II.78}$$

Proof. Let $D' := \mathcal{A}$, which is a linear space, due to $\mathcal{A}$ being a vector space. We can define the following map on it

$$\begin{aligned} (\ \ldots\ )\ :\ D' \times D' &\to \mathbb{C} \\ a \times b &\mapsto (a,b) := \omega(a^* b) \end{aligned} \tag{II.79}$$

which we will show to be a positive definite, symmetric, sesqui-linear form on D'. Using the polarisation identity [196]

$$a^* b = \frac{1}{4}\sum_{\epsilon^4 = 1} \bar{\epsilon}(a + \epsilon b)^*(a + \epsilon b) \tag{II.80}$$

with $\epsilon \in \{\pm 1, \pm i\}$, hence $\bar{\epsilon} = \epsilon^{-1}$ and $\bar{\epsilon}\epsilon = 1$. Then:

$$\begin{aligned} (a,b)^* = \omega(a^* b)^* = \left(\frac{1}{4}\sum_{\epsilon^4=1}\bar{\epsilon}\omega((a+\epsilon b)^*(a+\epsilon b))\right)^* = \frac{1}{4}\sum_{\epsilon^4=1}\epsilon\omega((a+\epsilon b)^*(a+\epsilon b)) = \\ = \frac{1}{4}\sum_{\epsilon^4=1}\epsilon\omega(\bar{\epsilon}\epsilon(b+\epsilon^{-1}a)^*(b+\epsilon^{-1}a)) = \frac{1}{4}\sum_{\epsilon^4=1}\bar{\epsilon}\omega((b+\epsilon a)^*(b+\epsilon a)) = \omega(b^* a) = (b,a) \end{aligned} \tag{II.81}$$

where we could neglect the outer involution in the third step due to positivity of ω and exchanged $\epsilon \leftrightarrow \bar{\epsilon}$ for the last line. Hence, $(.,.)$ is symmetric and obviously sesquilinear and non-negative by definition. However, it will in general have a non-vanishing kernel, hence consider:

$$\mathcal{N} = \{n \in D',\ \omega(n^* n) = 0\} \tag{II.82}$$

Then with $[a] = \{a + n,\ n \in \mathcal{N}\}$ and using (II.12)

$$\langle [a], [b]\rangle = \omega(a^* b) \tag{II.83}$$

is positive definite on $D := \{[a],\ a \in D'\}$. $\mathcal{N}$ is also a left-sided ideal, since for $a \in \mathcal{A},\ n \in \mathcal{N}$:

$$\omega((an)^* an) = (n, a^* an) = |(n, a^* an)| \leq (n,n)^{1/2}(a^* an, a^* an)^{1/2} = \omega(n^* n)(a^* an, a^* an)^{1/2} = 0 \tag{II.84}$$

using again Cauchy-Schwartz-inequality. So, we can choose as Hilbert space $\mathcal{H}$ the closure of D with respect to $\langle .,. \rangle$, as cyclic vector $\Omega := [1]$ and finally $\pi(a) = [a]$ for all $a \in \mathcal{A}$., which acts by $\pi(a)[b] = [ab]$. This is independent from the choice of representative as $\mathcal{N}$ is a left-ideal, so $a[b] = a(b+n) = ab + an$ with $an \in \mathcal{N}$. The linearity criterion for the representation of a $*$-algebra is obviously fulfilled, moreover:

$$\pi(ab)[c] = [abc] = \pi(a)[bc] = \pi(a)\pi(b)[c] \tag{II.85}$$

and

$$\langle [\pi(a)]^\dagger [b], [c]\rangle = \langle [b], \pi(a)[c]\rangle = \omega(b^* ac) = \omega((a^* b)^* c) = \langle \pi(a^*)[b], c\rangle \tag{II.86}$$

By definition of $\mathcal{H}$ we have D being dense and then $\pi(a)\Omega = [a \cdot 1] = [a]$ $\forall a \in \mathcal{A}$ shows that every point in D can be reached hence, Ω is a cyclic vector. To summarise we have indeed found a cyclic representation stemming from ω.
Consequently, given $(\pi, \mathcal{H}, \omega)$ equation (II.78) defines a state, if Ω is normalised, as

$$\langle \Omega, \pi(a^* a)\Omega\rangle = \langle \pi(a)\Omega, \pi(a)\Omega\rangle = ||\pi(a)\Omega||^2 \geq 0 \tag{II.87}$$

It remains to show uniqueness up to unitary equivalence. Assuming there would be another triple $(\pi', \mathcal{H}', \Omega')$, such that

$$\omega(a) = \langle \Omega, \pi(a)\Omega\rangle_{\mathcal{H}} = \langle \Omega', \pi'(a), \Omega'\rangle_{\mathcal{H}'} \tag{II.88}$$

which is a consequence of $\omega(a) = \omega(1^* a) = \langle [1], [a]\rangle_{\mathcal{H}} = \langle \Omega, \pi(a)\Omega\rangle_{\mathcal{H}}$. Then define

$$U: \ D \to D' \subset \mathcal{H}' \tag{II.89}$$
$$\pi(a)\Omega \mapsto \pi'(a)\Omega' \tag{II.90}$$

which is an isometry

$$\begin{aligned} ||U\pi(a)\Omega||^2_{\mathcal{H}} &= ||\pi'(a)\Omega'||^2_{\mathcal{H}'} = \langle \pi'(a)\Omega', \pi'(a)\Omega'\rangle_{\mathcal{H}'} = \langle \Omega', \pi'(a)^\dagger \pi'(a)\Omega'\rangle_{\mathcal{H}'} = \\ &= \langle \Omega', \pi'(a^* a)\Omega'\rangle_{\mathcal{H}'} = \omega(a^* a) = \ldots = ||\pi(a)\Omega||^2_{\mathcal{H}} \end{aligned} \tag{II.91}$$

Thus U is densely defined on D. And by the same calculation we find the existence of an $U^{-1} : D' \to D$. With $D' \subset \mathcal{H}'$, $D \subset \mathcal{H}$ both dense and $\mathcal{H}, \mathcal{H}'$ both closed, we can extend U, U^{-1} to a unitary operator according to the continuous linear extension theorem II.A.2, since isometry underlies boundedness. □

Dynamical Restrictions on the State ω

In the following, we impose restrictions on ω, which will allow us to implement time evolution in the quantum theory.

Definition II.B.2 (Automorphisms, G-invariance)**.** *Let G be a group, whose action on an algebra of observables $\mathcal{A}$ is given via* automorphism $\alpha_g: \ \mathcal{A} \to \mathcal{A}$ *with $g \in G$, i.e. maps obeying*

1. $\alpha_g \circ \alpha_{g'} = \alpha_{gg'}$ *for all* $g, g' \in G$
2. $\alpha_g(ab) = \alpha_g(a)\alpha_g(b)$ *and* $\alpha_g(a)^* = \alpha_g(a^*)$ $\forall a, b, \in \mathcal{A}$
3. $\alpha_g(z_1 a + z_2 b) = z_1 \alpha_g(a) + z_2 \alpha_g(b)$ $\forall z_1, z_2 \in \mathcal{C}$

We call G a symmetry *and a state ω in $\mathcal{A}$* G-invariant *iff* $\forall g \in G, \ a \in \mathcal{A}$

$$\omega(\alpha_g(a)) = \omega(a) \tag{II.92}$$

Lemma II.B.1. *Each G-invariant state ω leads to unitary representation of G on the GNS-Hilbert space corresponding to $\mathcal{A}, \omega$ by*

$$U(g)\,(\pi(a)\Omega) := \pi(\alpha_g(a))\Omega \tag{II.93}$$

for all $g \in G$. Moreover, Ω is a G-invariant vector in $\mathcal{H}$.

Proof. We show isometry of $U(g)$:

$$\langle U(g)\pi(a)\Omega, U(g)\pi(b)\Omega\rangle = \langle \pi(\alpha_g(a))\Omega, \pi(\alpha_g(b))\Omega\rangle = \langle \Omega, \pi(\alpha_g(a^*b))\Omega\rangle = \omega(\alpha_g(a^*b)) = \\ = \omega(a^*b) = ... = \langle \pi(a)\Omega, \pi(b)\Omega\rangle \tag{II.94}$$

Also $U(G)$ has as inverse $U(g^{-1})$, hence it can be extended to a unique unitary operator on the whole of $\mathcal{H}$. □

Physical input enters now in demanding that the vacuum Ω is a state which does *not* change under a global shift of the time coordinate, i.e. it gives rise to a G-invariant state ω with respect to the classical automorphism $\alpha_g^H(a) = \sum_n t^n/n!\{H,a\}_{(n)}$ induced by the Hamilton function H.
By the Stone theorem [194, 195] we have then guaranteed the existence of a self-adjoint operator $\hat{H} := \pi(H)$ as generator of time evolution. From (II.93) and setting $a = 1$ follows that it annihilates the vacuum

$$\hat{H}\Omega = 0, \qquad U(t) := \exp(-it\hat{H}) \tag{II.95}$$

In other words the vacuum is from now on referred to as a vector which does not change under time evolution, which we get automatically during the GNS construction.

The Stone-von Neumann Theorem

In special cases the choice of the states becomes unique. In this paragraph we will comment on when this happens.

Let us consider $\mathcal{S}(\mathbb{R}^n)$ the space of Schwartz functions, i.e. $f : \mathbb{R}^n \to \mathbb{R}$ which are of rapid decrease. In other words $f \in \mathcal{S}(\mathbb{R}^n)$ iff $\int_\sigma d^3x\, f(x)P(x) \leq \infty$ for any polynomial P. In the following we use its elements often as *test functions*.

Definition II.B.3 (Weyl Algebra)**.** *(cf. [197, 198]) The (spatial) Weyl elements of a scalar field theory are defined as ($f, g \in \mathcal{S}(\sigma)$)*

$$w[f,g](\phi,\pi) := \exp\left(i(\phi[f] + \pi[g])\right), \qquad w[f](\phi) := w[f,0](\phi,\pi) \tag{II.96}$$

Similarly the (spatial) Weyl elements for the phase space $\mathbb{R}^2$ of a mechanical system with $\{p,q\} = 1$ are ($x, y \in \mathbb{R}$)

$$w[x,y](q,p) := \exp\left(i(yq + xp)/\hbar\right) \tag{II.97}$$

The $*$-algebra generated by the finite linear combinations of some Weyl elements is called the Weyl algebra, $\mathcal{W}$. For each Weyl algebra, we define the maps $.^* : \Gamma \to \Gamma$ and $f_\alpha : \Gamma \times \Gamma \to \Gamma$ (where Γ is either $\mathcal{S}(\sigma)$ or $\mathbb{R}^2$) such that

$$w[f^*] := w[f]^*, \qquad w[f]w[f'] := \sum_{\alpha=1}^{L} z_\alpha w[f_\alpha(f,f')], \qquad \forall f, f' \in \Gamma \tag{II.98}$$

where $L < \infty$.

Example: For the scalar field theory, the Weyl relations (II.98) have the following, explicit form of the parameters ($f, f' \in \mathcal{S}(\sigma)$)

$$f^* = -f, \qquad L = 1, \qquad z_1 = 1, \qquad f_1(f,f') = f + f' \tag{II.99}$$

In case of a one particle system, the parameter of the relations read: ($x, y \in \mathbb{R}^2$)

$$(x_1,x_2)^* = (-x_1,-x_2), \quad L = 1, \quad z_1(x,y) = e^{\frac{-i}{2\hbar}(x_1y_2 - x_2y_1)}, \quad f_1(x,y) = (x_1 + x_2, y_1 + y_2) \tag{II.100}$$

Definition II.B.4. *A state ω on a Weyl algebra $\mathcal{W}$ is called* regular*, iff for the corresponding representation $(\pi, \mathcal{H})$ the 1-parameter groups $x_1 \mapsto \pi(w[x_1,0])$ and $x_2 \mapsto \pi(w[0,x_2])$ are strongly continuous, i.e.*

$$\lim_{x\to 0} ||(\pi(w[x,0]) - \mathbb{1}_\mathcal{H})\Psi|| = 0, \qquad \forall \Psi \in \mathcal{H} \tag{II.101}$$

and similar for the second argument of $w[.,.]$.

Theorem II.B.2 (Stone-von Neumann)**.** *(cf. [192–195]) Given the Weyl-algebra of a one-particle system, i.e. with finitely many degrees of freedom. Let ω be a state thereon, whose GNS representation $(\pi, \mathcal{H})$ is irreducible and with respect to which the Weyl elements $w[x,y]$ are regular.*
Then ω is equivalent to the Fock-state ω^l:

$$\omega(w[x,y]) = \omega^l(w[x,y]) := \exp\left(-\frac{1}{4}(\frac{x^2}{l^2} + \frac{y^2 l^2}{\hbar^2})\right) \tag{II.102}$$

with $l > 0$ and $[l]$ =cm.

For the proof of this theorem there are excellent accounts in the literature. See e.g. [199] for a modern version.

In the case of a field theory the Stone-von Neumann theorem is not applicable and other methods must be used to classify all possible states on $\mathcal{A}$. A formulation, which is used in constructive QFT and in terms of which the Gårding-Wightman axioms [163] are formulated, are the *Wightman functions*:

Definition II.B.5 (Wightman functions, Schwinger functions)**.** *Let $\mathcal{A}$ be an algebra of observables with state ω such that the Hamilton function H can be represented as a self-adjoint operator $\hat{H} = \pi(H)$ on $\mathcal{H}$. Moreover, we demand that $\pi(\mathcal{A})$ contains the* time-dependent Heisenberg fields

$$\hat{\phi}_I(p,t) = \exp(-it\hat{H})\hat{\phi}_I(p,0)\exp(it\hat{H}) \tag{II.103}$$

where $\hat{\phi}_I(p,0) := \pi(\phi_I(p))$ with $p \in \sigma$.
Then the Wightman n-point functions[12] *are defined as ($x_i \in \sigma \times \mathbb{R}$)*

$$\mathrm{W}_{n,I_n...I_1}(x_n,...,x_1) := \langle \Omega, \hat{\phi}_{I_n}(x_n)...\hat{\phi}_{I_1}(x_1)\Omega\rangle_{\mathcal{H}} \tag{II.104}$$

And their analytic continuations $t \mapsto i\beta$, $\beta \in \mathbb{R}$ will be called the Schwinger n-point functions S_n.

II.B.2 Path integral Quantisation of Euclidian fields

In this subsection we will be working in the covariant formulation, i.e. using the history time fields Φ_I rather than the canonical pair (ϕ_I, π_{ϕ_I}).
Most of the work in the previous section is side-stepped by simply defining a candidate for the Schwinger n-point function in the following way:

Definition II.B.6 (Euclidian functions)**.** *Given a field theory described by an action of the form*

$$S[\Phi_I] = S_0[\Phi_I] + V[\Phi_I] := \int_{\mathcal{M}} d^4x \; (\; \frac{1}{2}\sum_{I,\alpha}(\partial_\alpha \Phi_I)^2(x) + V(\{\Phi_I\}_I(x)) \;) \tag{II.105}$$

with S_0 the action of the free field and the semi-bounded potential $V[\Phi_I] \geq 0$.
Then the Euclidian n-point function *is defined as the path integral (or functional integral) [200]*

$$\mathrm{E}_{n,I_n...I_1}(x_n...x_1) = \int d\mu(\Phi)\; \Phi_{I_n}(x_n)...\Phi_{I_1}(x_1), \qquad d\mu(\Phi) = e^{-S_N[\Phi_I]/\hbar} \lim_{N\to\infty} \prod_{v\in T(1/N)} d\Phi(v) \tag{II.106}$$

with $\mu(1) = 1$ and $T(1/N)$ is some cubulation of $\mathcal{M}$ with cells of vanishing volume for $N \to \infty$.[13] *Lastly, $S_N[\Phi]$ is for all N bounded from below and some discretisation of the continuum action, such that $S[\Phi_I] = \lim_{N\to\infty} S_N[\Phi_I]$.*[14]

As we realise, the action $S[\Phi_I]$ is by definition bounded from below, it made sense to demand the same for $S_N[\Phi_I]$. Hence, the exponent $\exp(-S_N[\Phi_I])$ is bounded from above and strictly positive. Thus, $d\mu(\Phi)$ indeed defines a positive measure.

[12] Strictly speaking these objects (and all other n-point functions) are distributions, but we will stick to the notation commonly found in the literature.
[13] Note that the limit must be taken *before* evaluating the integral. This makes $d\mu(\Phi)$ a mathematically ill-defined object, known as the *Euclidian path integral measure*.
[14] We will encounter explicit examples for such discretisations in chapter *III. Renormalisation*.

Consequently, we can hope to identify the Euclidian n-point function with the Schwinger function of a canonical theory as they are fulfilling the same properties of a vacuum expectation value.

On the other hand, the set of possible actions of the form (II.105) should be too restrictive for all applications in mind (e.g., we will later consider the Einstein-Hilbert action of General Relativity). So we will allow more general measures, yet are then faced with the question, whether they give rise to a corresponding well-defined caonincal quantum theory. Sufficient conditions on the measure for this have been collected by Osterwalder and Schrader [135–137]. We now state the axioms and present the explicit construction in the following section.

Definition II.B.7 (Generating functional)**.** *Given a field theory on $\mathcal{M} \cong \sigma \times \mathbb{R}$, we perform a rotation to imaginary time $t \mapsto i\beta$, $\beta \in \mathbb{R}$. Fields on this space, $\mathcal{R}$, are called* Euclidian fields*.*
Consider the distribution space $\mathcal{S}'(\mathcal{R})$ on the Schwartz functions, such that $\Phi_I \in \mathcal{S}'(\mathcal{R})$ via

$$\Phi_I[F] = \langle \Phi_I, F\rangle_{\mathcal{R}} = \int_{\mathcal{R}} d^4x\ \Phi_I(x)F(x) \tag{II.107}$$

$\forall F \in \mathcal{S}(\mathcal{R})$ called test functions. For $F_I \in \mathcal{S}(\mathcal{R})$, $I = 1....N$, we define $W[F] : \mathcal{S}'(\mathcal{R}) \to \mathbb{C}$ with $W[F](\{\Phi_I\}) := \exp(i \sum_I \Phi_I[F_I])$ and

$$\mathfrak{A}_+ = \{\Psi(\ .\ ) = \sum_{K=1}^{N} z_K W[F^K](\ .\ )\ ,\ z_K \in \mathbb{C},\ \mathrm{T}-\mathrm{supp}(F_I^K) \subset (0,\infty)\} \tag{II.108}$$

Then, given a measure μ on $\mathcal{S}'(\mathcal{R})$, we define the generating functional of the Schwinger functions*:*

$$S[F] = \int_{\mathcal{S}'(\mathcal{R})} d\mu(\Phi)\ W[F](\Phi) \tag{II.109}$$

Definition II.B.8 (Osterwalder-Schrader axioms)**.** *The* OS axioms *are conditions which a measure μ (uniquely determined by its generating functional) may satisfy. They read explicitly:*

OS0 Analyticity. *For all $F^K \in \mathcal{S}(\mathcal{R})$, $K \leq N < \infty$ and $z_1...z_N \in \mathbb{C}$ the function*

$$\vec{z} \mapsto S[\sum_K z_K F^K] \tag{II.110}$$

is complex differentiable on the entire complex plane $\mathbb{C}^N$.[15]

OS1 Regularity. *There exists $1 \leq p \leq 2$ and $c \in \mathbb{C}$ such that for all $F \in \mathcal{S}(\mathcal{R})$ holds*[16]

$$|S[F]| \leq \exp\left(c(||F||_{L_1} + ||F||^p_{L_p})\right) \tag{II.111}$$

OS2 Euclidian invariance. *$S[F]$ is invariant under time reflections and translations. If $\mathcal{R} \cong \mathbb{R}^4$ then we might demand invariance under all Euclidian symmetries E, i.e. rotations and spatial reflections and translations:*[17]

$$S[F] = S[E\ F] \qquad \text{or equivalently} \qquad \mu(F) = \mu(E\ F) \tag{II.112}$$

OS3 Reflection positivity. *For the* time reflection *$R : \mathcal{S}'(\mathcal{R}) \to \mathcal{S}'(\mathcal{R})$, defined as $(R\Psi)(F) = \Psi(\theta F)$ with $\theta : \mathcal{S}(\mathcal{R}) \to \mathcal{S}(\mathcal{R})$ acting as $(\theta F)(x,t) = F(x,-t)$, the measure μ fulfils ($\forall \Psi \in \mathcal{E} := \overline{V}$, i.e. the closure of $V = \mathfrak{A}_+ \cap L_2(\mathcal{S}'(\mathcal{R}), d\mu)$)*[18]

$$0 \leq \langle \Psi, R\Psi\rangle_{\mathcal{E}} := \int d\mu(\Phi)\ \overline{\Psi(\Phi)}(R\Psi)(\Phi) \tag{II.113}$$

OS4 Cluster property:[19] *Let $F, F' \in \mathcal{S}(\mathcal{R})$, then holds*

$$\lim_{s\to\infty} \int d\mu(\Phi)\ \overline{W[F](\Phi)} W[T_s F'](\Phi) = \mu(\overline{W[F]})\mu(W[F']) = \langle W[F], 1\rangle_{\mathcal{E}} \langle 1, W[F']\rangle_{\mathcal{E}} \tag{II.114}$$

[15] In other words, $d\mu(\Phi)$ decays faster than any exponential. Dropping this axiom could force us to consider only a subset of all test functions.

[16] The L_p-norm is defined as $||.||_{L_p} :\ F \mapsto (\int |F(x)|^p dx)^{1/p}$.

[17] E.g. GR will provide counterexamples. Also note that, upon going back to Minkowski fields, this is equivalent to Lorentz invariance.

[18] This axiom guarantees positivity of the scalar product of a GNS Hilbert space and is therefore crucial for the subsequent constructions.

[19] This is slightly stronger than the *Ergodicity property* mentioned in [135]. However both ensure uniqueness of the vacuum.

II.C Bijection between OS measure and OS data

Given a field theory defined on a manifold $\mathcal{M} \cong \sigma \times \mathbb{R}$, for which we will consider a single field species. In this chapter we show that there is a unique one to one correspondence between a triple of *OS data* $(\mathcal{H}, \hat{H}, \Omega)$ (consisting out of a Hilbert space, a self-adjoint Hamiltonian operator thereon and a cyclic vector) and an *OS measure* μ satisfying a subset of the Osterwalder-Schrader axioms. Moreover, we will only consider scalar fields in the following, for extensions to gauge groups see [201–205].
For the Osterwalder-Schrader reconstruction we follow [128,135] and for the Osterwalder-Schrader construction and their inversion properties we quote the calculations from [128].

II.C.1 Osterwalder-Schrader Reconstruction

Let μ be a measure satisfying OS2 and OS3.
On V, the finite linear combinations of $W[F]$ with F of positive time support, we define the bi-linear form

$$\langle \Psi, \Psi' \rangle_V := \langle \Psi, R\Psi' \rangle_{\mathcal{E}} \tag{II.115}$$

which is positive by OS3, however not yet positive definite. Due to OS2 we have invariance under time reflections, giving sesqui-linearity of the form: (using unitarity of R)

$$\overline{\langle \Psi, \Psi' \rangle_V} = \langle R\Psi', \Psi \rangle_{\mathcal{E}} = \langle R^2\Psi', R\Psi \rangle_{\mathcal{E}} = \langle \Psi', \Psi \rangle_V \tag{II.116}$$

Lemma II.C.1. *Let μ be a measure on $\mathcal{S}'(\mathcal{R})$ satisfying OS3. Then the Null space*

$$\mathcal{N} = \{\Psi \in V,\ \langle \Psi, \Psi \rangle_V = 0\} \tag{II.117}$$

is a linear space. And upon defining the canonical Hilbert space $\mathcal{H}$ as the completion of the set $V/\mathcal{N}$ of equivalence classes $[\Psi] := \{\Psi + N,\ N \in \mathcal{N}\}$ with $\Psi \in V$, the scalar product

$$\langle [\Psi], [\Psi'] \rangle_{\mathcal{H}} := \langle \Psi, \Psi' \rangle_V \tag{II.118}$$

is well defined on $\mathcal{H}$, i.e. independent of the representative.

Proof. We need to show that if $\Psi, \Psi' \in V$ and $N \in \mathcal{N}$ then $\langle \Psi + N, \Psi' \rangle_{\mathcal{H}} = \langle \Psi, \Psi' \rangle_{\mathcal{H}}$. And from

$$\langle \Psi + N, \Psi' \rangle_{\mathcal{H}} = \int \overline{\Psi + N} R\Psi' = \langle \Psi, \Psi' \rangle_{\mathcal{H}} + \langle N, \Psi' \rangle_{\mathcal{H}} \tag{II.119}$$

follows with the Cauchy-Schwarz-inequality (II.12), which applies to positive definite sesqui-linear forms, that:

$$|\langle N, \Psi' \rangle_{\mathcal{H}}| \leq \langle N, N \rangle_{\mathcal{H}}^{1/2} \langle \Psi', \Psi' \rangle_{\mathcal{H}}^{1/2} = 0 \tag{II.120}$$

□

We define densely on $L_2 := L_2(\mathcal{S}'(\nabla), d\mu)$: $(s \in \mathbb{R})$

$$(T_s F)(\beta) := F(\beta - s), \qquad \mathcal{U}(s)W[F] := W[T_s F] \tag{II.121}$$

Note that $\mathrm{T} - \mathrm{supp}(T_s F) = \mathrm{T} - \mathrm{supp}(F) + s$ thus $\mathcal{U}(s)$ does not map V onto V unless $s > 0$. Thus, on V we may still define a one parameter family $s \mapsto \mathcal{U}(s)$ but it is a semi-group rather than a group, because its inverses are not defined.
We want to define for $\Psi \in V$

$$K(s)[\Psi] := [\mathcal{U}(s)\Psi] \tag{II.122}$$

but we must first show that this definition is well-defined, i.e. $\mathcal{U}(s)\mathcal{N} \subset \mathcal{N}$. For this note first that

$$(\theta\, T_s F)(\beta) = (T_s F)(-\beta) = F(-b - s) = (\theta F)(\beta + s) = (T_{-s}\, \theta F)(\beta) \tag{II.123}$$

whence $R\mathcal{U}(s)W[F] = W[\theta\, T_s F] = \mathcal{U}(-s)RW[F]$. Thus using unitarity of $\mathcal{U}(s)$ on L_2 for $\Psi \in V, N \in \mathcal{N}$

$$\begin{aligned}\langle R\mathcal{U}(s)N, \mathcal{U}(s)N \rangle_{L_2} &= \langle \mathcal{U}(-s)RN, \mathcal{U}(s)N \rangle_{L_2} = \langle RN, \mathcal{U}(2s)N \rangle_{L_2} \\ &\leq \langle RN, N \rangle^{1/2} \langle_{L_2} R\mathcal{U}(2s)N, \mathcal{U}(2s)N \rangle_{L_2}^{1/2} = 0\end{aligned} \tag{II.124}$$

hence giving the claim that $\mathcal{U}(s)\mathcal{N} \subset \mathcal{N}$.

Theorem II.C.1 (Reconstruction of canonical Quantum Theory)**.** *Let μ be a measure on $\mathcal{S}'(\mathcal{R})$ satisfying to OS2 and OS3. Then from (II.122) we have for $s \geq 0$*

$$K(s) = \exp\left(-s\hat{H}\right) \tag{II.125}$$

Here, $\hat{H} : \mathcal{S}'(\mathcal{R}) \to \mathcal{S}'(\mathcal{R})$ is a self-adjoint positive operator, i.e. $0 \leq \hat{H} = \hat{H}^\dagger$. Moreover, $\Omega := [1] = [W[F]|_{F=0}] \in \mathcal{S}'(\mathcal{R})$ is a ground state of $\hat{H}$, i.e.

$$\hat{H}\Omega = 0 \tag{II.126}$$

Proof. We verify the following four properties:
(i) Semigroup law: $K(t)K(s) = K(t+s)$, for all $s, t \in \mathbb{R}_+$. This follows from the multiplication law for $\mathcal{U}(s)$:

$$K(t)K(s)[\Psi] = [\mathcal{U}(s)\mathcal{U}(t)\Psi] = [\mathcal{U}(t+s)\Psi] = K(t+s)[\Psi] \tag{II.127}$$

(ii) $K(s)$ is self-adjoint, as

$$\begin{aligned}\langle[\Psi], K(s)[\Psi']\rangle_{\mathcal{H}} = \langle\Psi, R\mathcal{U}(s)\Psi'\rangle_{L_2} = \langle\Psi, \mathcal{U}(-s)R\Psi'\rangle_{L_2} = \int d\mu(\Phi)\overline{\Psi(\Phi[.])}(R\Psi')(\Phi[T_{-s}\,.]) = \\ = \langle\mathcal{U}(s)\Psi, R\Psi'\rangle_{L_2} = \langle K(s)[\Psi], [\Psi']\rangle_{\mathcal{H}}\end{aligned} \tag{II.128}$$

Moreover, $K(s)$ is positive as follows from

$$\langle[\Psi], K(s)[\Psi]\rangle_{\mathcal{H}} = \langle[\Psi], [\mathcal{U}(s/2)^2\Psi]\rangle_{\mathcal{H}} = \langle[\Psi], K(s/2)^2[\Psi]\rangle_{\mathcal{H}} = ||K(s/2)[\Psi]||^2_{\mathcal{H}} \tag{II.129}$$

(iii) $K(s)$ is a contraction, i.e. $||K(s)||_{\mathcal{H}} \leq 1$. For this we consider any $0 \neq [\Psi] \in \mathcal{H}$ then:

$$||K(s)[\Psi]||_{\mathcal{H}} = \sqrt{\langle[\Psi], K(s)^2[\Psi]\rangle_{\mathcal{H}}} \leq ||[\Psi]||^{1/2}_{\mathcal{H}}||K(2s)[\Psi]||^{1/2}_{\mathcal{H}} \leq ||[\Psi]||^{\sum_{k=1}^n 2^{-k}}_{\mathcal{H}}\ ||K(2^n s)[\Psi]||^{2^{-n}}_{\mathcal{H}} \tag{II.130}$$

And with $(r > 0)$

$$||K(r)[\Psi]||^2_{\mathcal{H}} = ||[\mathcal{U}(r)\Psi]||^2_{\mathcal{H}} = \langle\mathcal{U}(r)\Psi, R\mathcal{U}(r)\Psi\rangle_{L_2} \leq ||\mathcal{U}(r)\Psi||_{L_2}||R\mathcal{U}(r)\Psi||_{L_2} \leq ||\Psi||^2_{L_2} \tag{II.131}$$

we get for any $n \in \mathbb{N}$

$$||K(s)[\Psi]||_{\mathcal{H}} \leq ||[\Psi]||^{1-2^{-n}}_{\mathcal{H}}||\Psi||^{2^{-n}}_{L_2} \tag{II.132}$$

and taking the limit $n \to \infty$:

$$\frac{||K(s)[\Psi]||_{\mathcal{H}}}{||[\Psi]||_{\mathcal{H}}} \leq 1 \tag{II.133}$$

taking the supremum over $[\Psi] \neq 0$ shows that $K(s)$ is bounded by norm one.
(iv) Strong continuity: $K(s) \to \mathbb{1}$ as $s \to 0$. By assumption $\mathcal{U}(s)$ is reflection continuous whence

$$\begin{aligned}||(K(s) - \mathbb{1})[\Psi]||^2_{\mathcal{H}} = \langle\Psi, R(\mathcal{U}(2s) - 2\mathcal{U}(s) + \mathbb{1})\Psi\rangle_{L_2} \leq \\ \leq |\langle\Psi, R(\mathcal{U}(2s) - \mathbb{1})\Psi\rangle_{L_2}| + 2|\langle\Psi, R(\mathcal{U}(s) - \mathbb{1})\Psi\rangle_{L_2}| \underset{s\to 0}{\longrightarrow} 0\end{aligned} \tag{II.134}$$

These properties say that $K(s)$ is a strongly continuous, self-adjoint, contraction semigroup and then there exists an operator $\hat{H}$ such that $K(s) = \exp(-s\hat{H})$ by the Hille-Yosida theorem [206]. If we take the derivative of (II.128) with respect to s and set afterwards $s = 0$ we deduce moreover that $\hat{H}$ must be self-adjoint too. Furthermore $\mathcal{U}(s)\mathbb{1} = \mathbb{1}$ and then $\forall s > 0$:

$$K(s)\Omega = [\mathcal{U}(s)W[F]\ |_{F=0}] = [W[T_sF]\ |_{F=0}] = [1] = \Omega \tag{II.135}$$

so that Ω is a vacuum for $\hat{H}$. □

Lemma II.C.2 (Uniqueness of vacuum)**.** *The vacuum Ω is unique, if the measure μ obeys OS4, i.e. it is time-clustering.*

Proof. If (II.114) holds for all $W[F]$ (which are dense), then for $s \to \infty$ the operator $\mathcal{U}(s)$ becomes a projection operator

$$\lim_{s\to\infty} \mathcal{U}(s) = \langle 1, \ . \ \rangle_{L_2} 1 \tag{II.136}$$

Now suppose there are any Ω such that $K(s)\Omega = \Omega$. Then for all $[\Omega'] = \Omega$ we have

$$(K(s) - \mathbb{1}_{\mathcal{H}})\Omega = [(\mathcal{U}(s) - \mathbb{1}_{L_2})\Omega'] = 0 \tag{II.137}$$

In other words $(\mathcal{U}(s) - \mathbb{1}_{L_2})\Omega' \in \mathcal{N}$ for any s. If μ clusters then take $s \to \infty$ and find

$$\lim_{s\to\infty} (\mathcal{U}(s) - \mathbb{1}_{L_2})\Omega' = \langle 1, \Omega' \rangle 1 - \Omega' \in \mathcal{N} \tag{II.138}$$

i.e. $\Omega := [\Omega'] \sim [1]$ and the vacuum is unique up to a phase. □

II.C.2 Osterwalder-Schrader Construction

In this section, we follow [128]. Let $(\mathcal{H}, \hat{H}, \Omega)$ be a representation π of a $*$-algebra $\mathcal{A}$ of observables generated by the Weyl elements $w[f](\phi) := \exp(i\phi[f])$ that support the Hamiltonian as a self-adjoint operator. For the corresponding operators, we write $\hat{w}[f] := \pi(w[f]), \hat{\phi}[f] := \pi(\phi[f])$ unless stated otherwise. We define the *N-th Wightman function generator*[20] as

$$W^N\left((f_N, t_N), ..., (f_1, t_1)\right) := \langle \Omega, \hat{w}[f_N] U(t_N - t_{N-1})^{-1} ... U(t_2 - t_1)^{-1} \hat{w}[f_1]\Omega \rangle_{\mathcal{H}} \tag{II.139}$$

and correspondingly the *N-th Schwinger function generator* with $t \mapsto i\beta,\ \beta \in \mathbb{R}$ as

$$S^N\left((f_N, \beta_N), ..., (f_1, \beta_1)\right) := \langle \Omega, \hat{w}[f_N] e^{-(\beta_N - \beta_1)\hat{H}} ... e^{-(\beta_2 - \beta_1)\hat{H}} \hat{w}[f_1]\Omega \rangle_{\mathcal{H}} \tag{II.140}$$

where $\beta_N > ... > \beta_1$ and $\hat{H}$ is bounded from below. The Wightman functions from (II.104) can be obtained from (II.139) by taking the functional derivatives with respect to $f_1 ... f_N$ and then setting them to zero.
Now, we want to use the N-th Wightman function generator to define a measure candidate. For this, we need the spectrum of an abelian algebra:

Definition II.C.1 (Spectrum of an abelian C^*-algebra)**.** *Let $\mathfrak{B}$ an abelian C^*-algebra. The* spectrum, *called $\Delta(\mathfrak{B})$, of it are the $*$-homomorphisms $\chi : \mathfrak{B} \to \mathbb{C}$ such that*

$$\chi(ab) = \chi(a)\chi(b), \qquad \chi(a+b) = \chi(a) + \chi(b), \qquad \chi(a)^* = \chi(a^*) \tag{II.141}$$

Especially in the case of a scalar field, we consider the $w[f]$ as the algebra generated by them is surely abelian. Then, we promote it to a C^*-algebra by equipping it with the C^*-norm induced by the operator norm [186] and complete it with respect to it. Due to the $w[f]$ being bounded, this will be a sub algebra of $\mathcal{A}$ and we denote it with the symbol $\mathfrak{B}$ in the following. Due to the Gel'fand isomorphism, $\mathfrak{B} \cong \mathfrak{B}^\vee \subset C(\Delta(\mathfrak{B}))$. Hence, we can think of a representation $(\pi(\mathfrak{B}), \mathcal{H})$ in the following way: $\mathcal{H} \cong L_2(\Delta(\mathfrak{B}), d\nu')$ with some measure $d\nu'$ and $\pi(\mathfrak{B})$ as continuous functions on $\Delta(\mathfrak{B})$ acting by multiplication on $\mathcal{H}$. For further details see [128, 185–188, 207, 208].
Now, we simply define:

Definition II.C.2. *Let ν be the Hilbert space measure corresponding to $(\mathcal{H}, \hat{H}, \Omega)$ with $\hat{H}$ bounded from below and $B_k \subset \Delta(\mathfrak{B})$ the open sets with respect to ν. We define the* spacetime fields *Φ as the elements of the set $\Gamma := \{\Phi \mid \Phi(\beta_1) \in \Delta(\mathfrak{B}),\ \forall \beta_1 \in \mathbb{R}\}$. The* cylindrical sharp time subsets *of Γ are*

$$\Gamma^{\beta_1 ... \beta_N}_{B_1 ... B_N} := \{\Phi \in \Gamma \mid \Phi(\beta_k) \in B_k, k = 1, ..., N\} \tag{II.142}$$

where $\beta_1 < ... < \beta_N$ are real numbers. Then we assign to those sets the heat kernel measure *μ by*

$$\mu(\Gamma^{\beta_1, ..., \beta_N}_{B_1, ..., B_N}) := \langle \Omega, \chi_{B_N} e^{-(\beta_N - \beta_{N-1})\hat{H}} ... e^{-(\beta_2 - \beta_1)\hat{H}} \chi_{B_1}\Omega \rangle_{\mathcal{H}} \tag{II.143}$$

where χ_B is the operator that multiplies by the characteristic function $\chi_B(\phi), \phi \in \Delta(\mathfrak{B})$.

[20] If the Hamiltonian function H is quadratic in the momenta π_ϕ we have $\{H, \phi\} = \pi_\phi$ and by taking suitable limits of $\pi(\alpha^H_t(w[f](.)))$ we can reconstruct the canonical pair (ϕ, π_ϕ) from it. Hence, any scalar product can, in this case, be obtained from this generator.

One has to note that μ defined this way might not automatically be positive. Indeed there exist counter-examples for it [175], so we will restrict in the following to OS data for which Nelson-Symanzik [176] positivity can be ensured.
In the spirit of (II.40) we define the Lebesgue-integral by considering as simple functions the step functions

$$\chi_{\Gamma^{\{\beta_k\}}_{\{B_k\}}}(\Phi) := \prod_{k=1}^{N} \chi_{B_k}(\Phi(\beta_k)) \tag{II.144}$$

Definition II.C.3 (Functions of sharp time support)**.** *For a finite set of $f_k \in \mathcal{S}(\sigma)$, $k = 1...N$, we define the smearing functions of* sharp time support *as the (formal) objects*

$$F := \sum_{k=1}^{N} \delta_{\beta_k} f_k \tag{II.145}$$

depending on N many sharp time points β_k.
The time-dependent Weyl element of a function of sharp time support is then simply defined as

$$W[F] := \prod_{k=1}^{N} W[\delta_{\beta_k,.}, f_k], \qquad W[\delta_{\beta,.}f] := w[f] \mid_{\phi\to\Phi(\beta)} \tag{II.146}$$

i.e. the Weyl element with the time zero field $\phi(x)$ replaced by the history time field $\Phi(\beta, x)$.

Corollary II.C.1. *Let $W[F]$ with $F = \sum_k f_k \delta_{\beta_k,.}$ of finite sharp time support . Then with $\beta_N > ... > \beta_1$*

$$\mu(\prod_{k=1}^{N} W(\delta_{\beta_k} f_k)) = \langle\Omega, \hat{w}(f_N)e^{-(\beta_N-\beta_{N-1})\hat{H}}\hat{w}(f_{N-1}) \; ... \; e^{-(\beta_2-\beta_1)\hat{H}}\hat{w}(f_1)\Omega\rangle_{\mathcal{H}} \tag{II.147}$$

Proof. By defining $s(\Phi) := \sum z^{\{\beta_I\}}_{\{B_I\}}\chi^{\{\beta_I\}}_{\{B_I\}}(\Phi)$ we see that $z^{\{\beta_I\}} = 0$ unless $\{\beta_I\} = \{\beta_k\}$. Then we can use (II.143) and the fact that simple functions approximate the function pointwise to obtain the claim. Note also that due to the fact that Φ on the left hand side is just an integration variable, all $W[\delta_{\beta_k,.}f_k]$ commute with each other. □

Theorem II.C.2 (Osterwalder-Schrader Construction)**.** *Given the OS data $(\mathcal{H}, \hat{H}, \Omega)$ and knowledge of the Schwinger n-point functions. Then the measure candidate μ defined in (II.147) automatically satisfies OS2 (i.e. time reflection and time translation invariant) and OS3 (i.e. reflection positivity).*

Proof. Let $\mathcal{H}' := L_2(\Gamma, d\mu)$ be the closure of the linear span of the functions $W[F]$ equipped with the scalar product

$$\langle W[F], W[F']\rangle_{\mathcal{H}'} := \mu(\overline{W[F]}W[F']) \tag{II.148}$$

We remember that due to the defining properties of a Lie algebra representations (see II.A.7) we know the existence of f^*, f_α, z_α such that:

$$\hat{w}[f]^\dagger = \hat{w}[f^*], \qquad \hat{w}[f]\hat{w}[f'] = \sum_{\alpha=1}^{N} z_\alpha \hat{w}[f_\alpha(f, f')] \tag{II.149}$$

and (as before in OS reconstruction) define densely the operators on $\mathcal{H}'$.

$$(RW)[F] := W[\theta F], \qquad (\theta F)(x, \beta) = F(x, -\beta) \tag{II.150}$$

This operator is unitary as can be seen, since for $F(t) = \sum_k \delta_{\beta_k,t} f_k$ with $\beta_1 < ... < \beta_N$ we have $(\theta F)(t) = \sum_k \delta_{-\beta,t} f_k$ whence due to $-\beta_N < ... < -\beta_1$:

$$\begin{aligned}\mu(R\, W[F]) &= \langle\Omega, \hat{w}[f_1]e^{-(-\beta_1+\beta_2)\hat{H}}\hat{w}[f_2]e^{-(-\beta_2+\beta_2)\hat{H}} \; ... \; e^{-(\beta_{N-1}+\beta_N)\hat{H}}\hat{w}[f_N]\Omega\rangle_{\mathcal{H}} = \\ &= \langle\hat{w}[f_N]^\dagger e^{-(\beta_N-\beta_{N-1})\hat{H}} \; ... \; e^{-(\beta_2-\beta_1)\hat{H}} w[f_1]^\dagger\Omega, \Omega\rangle_{\mathcal{H}} = \\ &= \overline{\langle\Omega, \hat{w}[f_N^*]e^{-(\beta_N-\beta_{N-1})\hat{H}} \; ... \; e^{-(\beta_2-\beta_1)\hat{H}}\hat{w}[f_1^*]\Omega\rangle_{\mathcal{H}}} = \\ &= \overline{\mu(W[F^*])} = \int d\mu(\Phi)\; \overline{W[F^*]}(\Phi) = \mu(W[F^*]^*) = \mu(W[F])\end{aligned} \tag{II.151}$$

where we used positivity of the measure for the first equality of the last line. In the representation from Definition II.C.2 the $\hat{\phi}$ became multiplication operators and hence $w[f]^*(\phi) = \overline{w[f](\phi)}$ which translates to the $W[F]$. Hence, R is a unitary operator on $\mathcal{H}'$, consequently $R^2 = \mathbb{1}_{\mathcal{E}'}$ and μ is time reflection invariant.
Time translation invariance follows after defining

$$(T_s F)(\beta') := F(\beta' - s), \qquad \mathcal{U}(s)W[F] := W[T_s F] \tag{II.152}$$

Thus for F of finite time support $\{\beta_k\}$ as before, we deduce that $(T_s F)$ has support $\beta'_k = \beta_k + s$ and then (since $\beta'_k - \beta'_l = \beta_k - \beta_l$)

$$\mu(\mathcal{U}(s)W[F]) = \langle \Omega, \hat{w}[f_N] e^{-(\beta'_N - \beta'_{N-1})\hat{H}} \ldots e^{-(\beta'_2 - \beta'_1)\hat{H}} \hat{w}[f_1]\Omega \rangle_{\mathcal{H}'} = \mu(W[F]) \tag{II.153}$$

We continue by showing that the measure μ is automatically reflection positive on $V := \mathfrak{A}_+ \cap \mathcal{H}'$, i.e. $\langle \Psi, R\Psi \rangle_{\mathcal{H}'} \geq 0, \ \forall \Psi \in V$. Note that if $\mathrm{T} - \mathrm{supp}(F) \subset (0, \infty)$ then $\mathrm{T} - \mathrm{supp}(\theta F) \subset (-\infty, 0)$. Thus by definition of $\mathfrak{A}_+$ (see (II.108))

$$\begin{aligned}
\langle \Psi, R\Psi \rangle_{\mathcal{H}'} &= \sum_{IJ} \bar{z}_I z_J \mu(\overline{W[F]} W[\theta\, F]) = \sum_{I,J} \bar{z}_I z_J \mu(W[F^*] W[\theta\, F]) = \\
&= \sum_{I,J} \bar{z}_I z_J \langle \Omega, \hat{w}[f^{I*}_{N^I}] \ldots e^{-(\beta^I_2 - \beta^I_1)\hat{H}} \hat{w}[f^{I*}_1] e^{-(\beta^I_1 + \beta^J_1)\hat{H}} \hat{w}[f^J_1] e^{-(\beta^J_2 - \beta^J_1)\hat{H}} \ldots \hat{w}[f^J_{N^J}]\Omega \rangle_{\mathcal{H}'} = \\
&= \sum_{I,J} \bar{z}_I z_J \langle e^{-\beta^I_1 \hat{H}} \hat{w}[f^I_1] \ldots e^{-(\beta^I_{N^I} - \beta^I_{N^I - 1})\hat{H}} \hat{w}[f^I_{N^I}]\Omega, e^{-\beta^J_1 \hat{H}} \hat{w}[f^J_1] \ldots e^{-(\beta^J_{N^J} - \beta^J_{N^J-1})\hat{H}} \hat{w}[f^J_{N^J}]\Omega \rangle \\
&= || \sum_I z_I e^{-\beta^I_1 \hat{H}} \hat{w}[f^I_1] e^{-(\beta^I_2 - \beta^I_1)\hat{H}} \ldots e^{-(\beta^I_{N^I} - \beta^I_{N^I-1})\hat{H}} \hat{w}[f^I_{N^I}]\Omega ||^2_{\mathcal{H}'}
\end{aligned} \tag{II.154}$$

which is manifestly non-negative. □

II.C.3 OS Reconstruction and Construction are Inverses

Having Osterwalder-Schrader reconstruction and construction at hand, one can traverse freely between the measure theoretic formalism and the canonical description. Although the physical predictions will by definition not change, it is not clear, that if we e.g. started with a measure μ - after going through both algorithms - do not obtain only an equivalent measure μ' to μ. In this section we want to demonstrate that for a special class of theories both processes are indeed inverses. This class is characterised by an assumption, which we can formulate in two different ways:
1. Starting with the OS data, the $w[f](\hat{\phi})\Omega$ lie dense in the canonical Hilbert space $\mathcal{H}$.
2. Starting with the OS measure, the path integral fields at a fixed time are of the same form as the canonical configuration operator fields $W[\delta_{\beta_k,.}f] = w[f](\Phi(\beta_k))$.
Indeed, these two conditions turn out to be equivalent, as 2. gives 1. automatically during the OS reconstruction and we will show below, that starting with 1. we can always find an equivalent measure, such that 2. holds.

We repeat the steps from [128] and begin with the *reproduction of the OS data*, i.e. starting with $(\mathcal{H}, \hat{H}, \Omega)$ we ask if the reconstruction of the newly obtained measure μ recovers the original OS data. For all $\Psi \in V := \mathfrak{A}_+ \cap \mathcal{H}'$, i.e. $\Psi = \sum_J z_J W[F_J]$ we know from (II.154) that

$$|| \, [\Psi] \, ||^2_{V/\mathcal{N}} = || \sum_I z_I e^{-\beta^I_1 \hat{H}} \hat{w}[f^I_1] e^{-(\beta^I_2 - \beta^I_1)\hat{H}} \ldots e^{-(\beta^I_{N^I} - \beta^I_{N^I-1})\hat{H}} \hat{w}[f^I_{N^I}]\Omega ||^2_{\mathcal{H}} \tag{II.155}$$

and we will call

$$\psi := \sum_I z_I e^{-\beta^I_1 \hat{H}} \hat{w}[f^I_1] e^{-(\beta^I_2 - \beta^I_1)\hat{H}} \ldots e^{-(\beta^I_{N^I} - \beta^I_{N^I-1})\hat{H}} \hat{w}[f^I_{N^I}]\Omega \tag{II.156}$$

Since by assumption 1. the finite linear span of the $\hat{w}[f]\Omega$ lies dense in $\mathcal{H}$ for any $\epsilon > 0$ we find $\psi^\epsilon = \sum_J c_J \hat{w}[g^J]\Omega$ such that $||\psi - \psi^\epsilon||_{\mathcal{H}} < \epsilon$. Consider the corresponding $\Psi^\epsilon = \sum_J c_J W[\delta_{0,.} g^J]$. Then by the same calculation as in (II.154)

$$||[\Psi] - [\Psi^\epsilon]||^2_{V/\mathcal{N}} = ||\psi - \psi^\epsilon||^2_{\mathcal{H}} < \epsilon^2 \tag{II.157}$$

Since the scalar product on $\mathcal{H}$ is non-degenerate, by definition of the OS data, this demonstrates that the equivalence class of $[\Psi]$ can be labelled by representatives which lie in the closure of the span of the $W[F]$ with $F = \delta_{0,.}f$.
We wish to show that $\overline{V/\mathcal{H}}$ is isomorphic to $\mathcal{H}$ for which we define the embedding

$$\begin{aligned} E: \qquad \mathcal{H} \qquad\qquad &\to V \\ \psi = \sum_I z_I \hat{w}[f^I]\Omega \mapsto \Psi &= \sum_I z_I W[\delta_{0,.}f^I] \end{aligned} \tag{II.158}$$

It follows that $E(\Omega) = 1$ the constant function equal unity and the scalar products are isometric $||E(\psi)||_{\overline{V/\mathcal{N}}} = ||\psi||_{\mathcal{H}}$, i.e. $[E(\psi)]$ can be identified with ψ and we conclude $\overline{V/\mathcal{N}} = \mathcal{H}$.
It remains to show that the Hamiltonian remains unchanged, for which we consider (II.155) for F of finite time support $0 < \beta_1 < ... < \beta_N$

$$[W[F]] \equiv e^{-\beta_1 \hat{H}} \hat{w}[f_1] e^{-(\beta_2-\beta_1)\hat{H}} \hat{w}[f_2] \, ... \, e^{-(\beta_N - \beta_{N-1})\hat{H}} \hat{w}[f_N]\Omega \tag{II.159}$$

We use this to compute the contraction semi-group for $\psi = \sum_I z_I w[f^I]\Omega$

$$\hat{K}(s)\psi \equiv K(s)[E(\psi)] = [\mathcal{U}(s)E(\psi)] = [\sum_I z_I W[\delta_{s,.}f^I]] \equiv \sum_I z_I e^{-s\hat{H}} \hat{w}[f^I]\Omega = e^{-s\hat{H}}\psi \tag{II.160}$$

$\forall \psi \in \mathcal{H}$ hence indeed $\hat{K}(s) = e^{s\hat{H}}$ and we reconstructed again exactly the original OS data $(\mathcal{H}, \hat{H}, \Omega)$.

Now we turn to the *reproduction of the OS measure* where we ask whether the OS data ($\mathcal{H} = \overline{V/\mathcal{N}}$, $\Omega = [1]$, $\hat{H} = -[d/ds]_{s=0}K(s)$) stemming from a measure μ yield under OS construction as measure μ' again the original OS measure. According to assumption 2. the Weyl operators $\hat{w}[f]$ can be defined as multiplication operators on the Hilbert space, i.e. the equivalences classes of the temporal $W[G]$, explicitly

$$\hat{w}[f][W[G]] = [W[\delta_{0,.}f]W[G]] \tag{II.161}$$

This action is independent on the choice of representative, as for $[\Psi] = 0$ follows (using $\theta\delta_{0,.} = \delta_{0,.}$)

$$\begin{aligned} ||\hat{w}[f][\Psi]||^2_{\mathcal{H}} &= \langle W[\delta_{0,.}f]\Psi, R\, W[\delta_{0,.}f]\Psi\rangle_{\mathcal{H}'} = \langle W[\delta_{0,.}f]\Psi, W[\delta_{0,.}f](R\Psi)\rangle_{\mathcal{H}'} = \\ &= \langle \hat{w}[f]^\dagger \hat{w}[f][\Psi], [\Psi]\rangle_{\mathcal{H}} \leq ||\hat{w}[f]^\dagger \hat{w}[f][\Psi]||_{\mathcal{H}} ||[\Psi]||_{\mathcal{H}} = 0 \end{aligned} \tag{II.162}$$

by the Cauchy-Schwarz inequality (II.12).
We compute for F of discrete time support at $\beta_1 < ... < \beta_N$:

$$\begin{aligned} \mu'(W[F]) &= \langle \Omega, \hat{w}[f_N]K(\beta_N - \beta_{N-1})...K(\beta_2 - \beta_1)\hat{w}[f_1]\Omega\rangle_{\mathcal{H}} = \\ &= \langle \Omega, \hat{w}[f_N]K(\beta_N - \beta_{N-1})...K(\beta_2 - \beta_1)[W[\delta_{0,.}f_1]\cdot 1]\rangle_{\mathcal{H}} = \\ &= \langle , \hat{w}[f_N]K(\beta_N - \beta_{N-1}...\hat{w}[f_2][\mathcal{U}(\beta_2 - \beta_1)W[\delta_{0,.}f_1]]\rangle_{\mathcal{H}} = \\ &= \langle \Omega, \hat{w}[f_N]K(\beta_N - \beta_{N-1}..K(\beta_3 - \beta_2)[W[\delta_{0,.}f_2]W[\delta_{\beta_2-\beta_1,.}f_1]]\rangle_{\mathcal{H}} = \\ &= \langle \Omega, \hat{w}[f_N]K(\beta_N - \beta_{N-1})...\hat{w}[f_3][W[\delta_{\beta_3-\beta_2,.}f_2]W[\delta_{\beta_3-\beta_1,.}f_1]]\rangle_{\mathcal{H}} = \\ &= \langle [1], [W[\delta_{\beta_N-\beta_N,.}f_N]...W[\delta_{\beta_N-\beta_1,.}f_1]]\rangle_{\mathcal{H}} = \langle 1, RW[\delta_{\beta_N-\beta_N,.}f_N]...W[\delta_{\beta_N-\beta_1,.}f_1]\rangle_{\mathcal{H}'} = \\ &= \langle 1, W[\delta_{\beta_N-\beta_N,.}f_N]...W[\delta_{\beta_1-\beta_N,.}f_1]\rangle_{\mathcal{H}'} = \langle \mathcal{U}(\beta_N)\cdot 1, W[\delta_{\beta_N,.}f_N]...W[\delta_{\beta_1,.}f_1]\rangle_{\mathcal{H}'} = \\ &= \langle 1, W[F]\rangle_{\mathcal{H}'} = \mu(W[F]) \end{aligned} \tag{II.163}$$

thus indeed the measure coincides with μ.

II.D Example: Free scalar field

Due to the rather involved nature of the previous chapters, we will now study a concrete example. This will put the formalism developed so far into action and present how calculations therein are explicitly performed. The example which we will study is the *massive, free scalar field*, i.e. there are no interactions of any type. This limits the physical interest of this system as any phenomenon in our everyday live is described by interacting processes. However, as in this model all steps can be carried out analytically, it serves as good test case which

has been studied amongst others in [128]. We repeat the calculations from there.
The class of actions of a free field theory of mass m is given by

$$S_\phi = \int_{\mathcal{M}} \mathcal{L} := \frac{-1}{2\kappa_\phi}\int_{\mathcal{M}} dtd^Dx\ (\sqrt{-g}g^{\mu\nu}(\partial_\mu\phi)(\partial_\nu\phi) + \frac{\alpha}{2}\phi m^2\phi) \tag{II.164}$$

where α is a constant such that the dimensions match, hence we will denote in the following $p^2 := \alpha m^2$, the inverse Compton wave length of dimension $[\mathrm{cm}^{-2}]$. In order to make ϕ^2 dimensionless we have introduced the constant κ_ϕ. We specialise to $\mathcal{M} = \mathbb{R}^{D+1}$ and flat Minkowski spacetime $g_{\mu\nu} = \eta_{\mu\nu}$ with $\eta = -c^2dt^2 + d\bar{x}^2$. Then with $g^{00} = -1/c^2$ and $\sqrt{-g} = c$ follows (using integration by parts)

$$S_\phi = \frac{1}{2\kappa_\phi}\int_{\mathbb{R}^{D+1}} dtd^Dx\ (\frac{1}{c}\dot\phi^2 - c\phi(-\Delta + p^2)\phi) =: \frac{1}{2\kappa_\phi}\int_{\mathbb{R}^{D+1}} dtd^Dx\ (\frac{1}{c}\dot\phi^2 - c\phi\omega^2\phi) \tag{II.165}$$

where $\Delta = \sum_{a=1}^D (\partial/\partial x^a)^2$ is the Laplacian. We perform a Legendre transformation and with the canonical momentum $\pi_\phi := \partial\mathcal{L}/\partial\dot\phi = \dot\phi/(\kappa_\phi c)$ obtain the Hamiltonian density

$$H := \int d^Dx\ (\pi_\phi\dot\phi - \mathcal{L}) = \frac{1}{2}\int d^Dx\ (\kappa_\phi c\pi^2 + \frac{c}{\kappa_\phi}\phi\omega^2\phi) \tag{II.166}$$

II.D.1 Canonical Quantisation

The first step in the GNS construction was the choice of a suitable algebra of observables, $\mathcal{A}$, for which we have to choose a sub set $\mathcal{E} \subseteq C^\infty(\mathcal{F})$. Having in mind that we will also want to incorporate time evolution we will want to allow for a representation including the Hamiltonian function $\pi(H)$.
We choose the following set

$$\mathcal{E} := \{1, a[f], \overline{a[g]}, H \mid a := \frac{1}{\sqrt{2\hbar\kappa_\phi}}(\sqrt{\omega}\phi - i\kappa_\phi\frac{1}{\sqrt{\omega}}\pi)\ ,\ \forall f,g \in \mathcal{S}\} \tag{II.167}$$

Indeed, with ϕ and π being real so is the Hamiltonian and property 1 of Def II.B.1 is fulfilled. Since we can by addition respectively subtraction reconstruct ϕ, π_ϕ, $\mathcal{E}$ is for sure separating points as demanded in property 3. Also we check property 2, i.e. closure with respect to the Poisson bracket. For this (using integration by parts to shift the ω and $\{\pi(x), \phi(y)\} = \delta^D(x,y)$)

$$\begin{aligned}
\{a[f], \overline{a[g]}\} &= \frac{1}{2\hbar\kappa_\phi}\int d^Dxd^Dy\ \bar{f}(x)g(y)\{(\sqrt{\omega}\phi)(x) - (\frac{i\kappa_\phi}{\sqrt{\omega}}\pi)(x), (\sqrt{\omega}\phi)(y) + (\frac{i\kappa_\phi}{\sqrt{\omega}}\pi)(y)\} = \\
&= \frac{i\kappa_\phi}{2\hbar\kappa_\phi}\int d^Dxd^Dy\left((\frac{1}{\sqrt{\omega}}\bar{f})(x)(\sqrt{\omega}g)(y)\{\pi(x),\phi(y)\} + (\frac{1}{\sqrt{\omega}}g)(y)(\sqrt{\omega}\bar{f})(x)\{\phi(x),\pi(y)\}\right) \\
&= \frac{1}{i\hbar}\langle f, g\rangle_{L_2} \sim 1 \in \mathcal{E} && \text{(II.168)} \\
\{H, a[f]\} &= \hbar c\int d^Dx\{\bar{a}(x), a[f]\}(\omega a)(x) = ic\ a[\omega f] \in \mathcal{E} && \text{(II.169)}
\end{aligned}$$

where we used that

$$H = \hbar c\int d^Dx\ \overline{a}(x)(\omega a)(x) \tag{II.170}$$

With $\mathcal{E}$ defined in such a way we can construct the algebra of observables $\mathcal{A}$ and define as state on this algebra

$$\omega(b\ a[f]) = \omega((a[f])^* b) = 0 \tag{II.171}$$

$\forall b \in \mathcal{A},\ f \in \mathcal{S}$. Note that $(a[f])^* \in \mathcal{A}$ is defined via the involutive structure of the non-commutative $*$-algebra. Indeed (II.171) defines the action of ω on all polynomials of a, a^* and hence on all of $\mathcal{A}$, as other terms can be evaluated via knowing that $\omega(\mathbb{1}_\mathcal{A}) = 1$ by definition and that by (II.75) the commutator is proportional to the Poisson bracket: for a as an object in $\mathcal{A}$

$$[a[f], (a[g])^*] = \langle f, g\rangle_{L_2}\mathbb{1}_\mathcal{A} \tag{II.172}$$

Moreover, this state is invariant under the automorphism induced by H and can be used to implement the dynamics. Hence upon performing the GNS construction we know that the cyclic vector Ω must obey $\pi(H)\Omega = 0$ and due to (II.171) also

$$\hat{a}[f]\Omega := \pi(a[f])\Omega = 0 \tag{II.173}$$

This fact motivates to pick as operator for the Hamiltonian simply

$$\hat{H} := \hbar c \int d^D x \; \hat{a}^\dagger \omega \hat{a} \tag{II.174}$$

Expressing $\hat{H}$ again in terms of $\hat{a}, \hat{a}^\dagger$, which we will call *annihilation and creation operators*, bears the significant advantage that knowing the vacuum expectation values of all polynomials in those $\hat{a}, \hat{a}^\dagger$ operators, determines also all Wightman functions. Moreover, from $\hat{a}[f]\Omega = 0$ follows that

$$\mathcal{H} \equiv \bar{V}, \qquad V = span\left\{a^\dagger[f_N]...a^\dagger[f_1]\Omega, \;\; f_1...f_N \in \mathcal{S}(\mathbb{R}^D), \; N < \infty\right\} \tag{II.175}$$

Upon introducing the Weyl elements $f \in \mathcal{S}(\mathbb{R}^D)$

$$w[f] := \exp\left(i\hat{\phi}[f]\right) \tag{II.176}$$

(where $\hat{\phi}$ is defined by inverting (II.167)) we find that the monomials in $\hat{a}^\dagger[f]...\Omega$ are obtained via multiple functional derivatives on $w[f]$ and using that $\hat{a}[f]\Omega = 0$ for all f. Thus $\mathcal{H}$ is indeed generated by the field dependent Weyl elements.
Lastly, to determine the Hilbert space measure we need only to consider the mentioned Weyl elements: using the Baker-Campbell-Hausdorff (BCH) formula [209–211]

$$\nu(w[f]) := \langle \Omega, \hat{w}[f]\Omega\rangle_{\mathcal{H}} = \langle \Omega, \exp\left(i\sqrt{\frac{\hbar\kappa_\phi}{2}}(\hat{a}[\frac{1}{\sqrt{\omega}}f] + \hat{a}^\dagger[\frac{1}{\sqrt{\omega}}f])\right)\Omega\rangle_{\mathcal{H}} = e^{-\frac{\hbar\kappa_\phi}{4}\langle f,\omega^{-1}f\rangle_{L_2}} \tag{II.177}$$

which displays ν as a Gaussian measure. Indeed, using the easily verified Weyl relation for a scalar field, i.e. $w[f]w[g] = w[f+g], \; w[f]^* = w[-f]$, we can compute any expectation value.[21]
We present, as an example, the time evolution of vectors of the form $\exp(i\hat{\phi}[f])\Omega$ (which also span $\mathcal{H}$). For this, we use again the BCH formula

$$e^{-\beta\hat{H}/\hbar}\hat{a}[f]e^{\beta\hat{H}/\hbar} = \sum_{m=0}^{\infty}\frac{1}{m!}[-\beta\hat{H}/\hbar, \hat{a}[f]]_{(m)} = a[e^{\beta c\omega}f] \tag{II.178}$$

And similar for $\hat{a}^\dagger[f]$ gives

$$e^{-\beta\hat{H}/\hbar}\hat{\phi}[f]e^{\beta\hat{H}/\hbar} = \hat{a}[\sqrt{\frac{\hbar\kappa_\phi}{2\omega}}e^{\beta c\omega}f] + \hat{a}^\dagger[\sqrt{\frac{\hbar\kappa_\phi}{2\omega}}e^{-\beta c\omega}f] = \hat{\phi}[e^{-\beta c\omega}f] + \hat{a}[\sqrt{\frac{2\hbar\kappa_\phi}{\omega}}\mathrm{sh}(\beta c\omega)f] \tag{II.179}$$

Thus the time evolution of the vector $\exp(i\hat{\phi}[f])\Omega)$ is obtained:

$$\begin{aligned} e^{-\beta\hat{H}/\hbar}e^{i\hat{\phi}[f]}\Omega &= e^{i\hat{\phi}[e^{-\beta c\omega}f] + i\hat{a}[\sqrt{\frac{2\hbar\kappa_\phi}{\omega}}\mathrm{sh}(\beta c\omega)f]}\Omega = e^{-\frac{1}{2}[\hat{\phi}[e^{-\beta c\omega}f],\hat{a}[\sqrt{\frac{2\hbar\kappa_\phi}{\omega}}\mathrm{sh}(\beta c\omega)f]]}e^{i\hat{\phi}[e^{-\beta c\omega}f]}\Omega = \\ &= e^{\frac{\hbar\kappa_\phi}{4}(\langle f,\omega^{-1}f\rangle - \langle f, e^{-2\beta c\omega}\omega^{-1}f\rangle)}e^{i\hat{\phi}[e^{-\beta c\omega}f]}\Omega \end{aligned} \tag{II.180}$$

II.D.2 Constructing the Measure from the Hamiltonian Formulation

Via the above canonical quantisation, the Hilbert space $\mathcal{H}$ is the span of the $\hat{a}^\dagger[f_1]...\hat{a}^\dagger[f_N]\Omega$ and hence equivalently the span of the $\hat{w}[f]\Omega$.
As the spectrum of $\mathcal{A}$ are the real-valued distributions, we define as in [128] the spacetime fields as $\Phi(\beta) \in \Delta(\mathcal{A}) = \mathcal{S}'(\mathbb{R}^D)$. Hence $\Phi \in \Gamma = \mathcal{S}'(\mathbb{R}^{D+1})$. By the OS construction defined above the measure μ is defined for

$$W[F] := e^{i\Phi[F]}, \qquad F(\beta, x) = \sum_{k=1}^{N}\delta(\beta,\beta_k)f_k(x) \tag{II.181}$$

with $\beta_{k+1} > \beta_k$ and $f_k \in \mathcal{S}(\mathbb{R}^D)$, as being (see Definition II.143)

$$\mu(W[F]) := \langle \Omega, \hat{w}[f_N]e^{-(\beta_N-\beta_{N-1})\hat{H}/\hbar}...e^{-(\beta_2-\beta_1)\hat{H}/\hbar}\hat{w}[f_1]\Omega\rangle_{\mathcal{H}} \tag{II.182}$$

[21] The strategy is to first revert the vacuum expectation value of a monomial involving $\hat{\phi}$ and $\hat{\pi}$ into a polynomial in $\hat{a}^\dagger$, relate each term by functional derivatives to a product in Weyl elements and lastly combine them to a single one, whose measure is computed above.

In the remainder of this paragraph we will focus on finding an explicit expression for this object.
We start by expressing

$$e^{iz[f,\beta]} := e^{-\beta \hat{H}/\hbar} \hat{w}[f] e^{\beta \hat{H}/\hbar} \tag{II.183}$$

which implies

$$z[f,\beta] = e^{-\beta \hat{H}/\hbar} \phi[f] e^{\beta \hat{H}/\hbar} = \hat{\phi}[\mathrm{ch}(\beta c\omega) f] - i\hat{\pi}[\mathrm{sh}(\beta c\omega) \frac{\kappa_\phi}{\omega} f] \tag{II.184}$$

where we used Baker-Campbell-Hausdorff $e^A B e^{-A} = \sum_m [A,B]_{(m)}/m!$ and

$$[\hat{H}, \hat{\phi}[f]] = c\kappa_\phi i\hbar \pi[f], \qquad [\hat{H}, \hat{\pi}[f]] = -\frac{c}{\kappa_\phi} i\hbar \hat{\phi}[\omega^2 f] \tag{II.185}$$

Due to (II.182) involving multiple products of these we note:

Lemma II.D.1. *Let* $z_k := z(f_k, \beta_N - \beta_k)$ *then*

$$e^{iz_N} ... e^{iz_2} e^{iz_1} = e^{i \sum_{k=1}^N z_k} e^{\frac{1}{2} \sum_{k=2}^N \sum_{l=1}^{k-1} [z_k, z_l]} \tag{II.186}$$

and

$$\langle \Omega, e^{i \sum_{k=1}^N z_k} \Omega \rangle_{\mathcal{H}} = e^{\frac{\hbar \kappa_\phi}{2} \int_{\beta_1}^{\beta_N} ds ds' \langle F(s), \frac{e^{c(s-s')\omega}}{\omega} F(t) \rangle} \tag{II.187}$$

$$\langle \Omega, e^{\frac{1}{2} \sum_{k=2}^N \sum_{l=1}^{k-1} [z_k, z_l]} \Omega \rangle_{\mathcal{H}} = e^{-\frac{\hbar \kappa_\phi}{2} \int_{\beta_1}^{\beta_N} ds \int_{\beta_1}^{s} ds' \, \langle \mathrm{sh}(c(s-s')\omega) F(s), \frac{1}{\omega} F(s') \rangle} \tag{II.188}$$

Proof. By the BCH formula

$$\begin{aligned} e^{iz_N} ... e^{iz_1} &= e^{iz_N} ... e^{iz_3} e^{i(z_1+z_2)} e^{\frac{1}{2}[z_2,z_1]} = e^{iz_N} ... e^{iz_4} e^{i(z_1+z_2+z_3)} e^{\frac{1}{2}([z_2,z_1]+[z_3,z_1+z_2])} \\ &= e^{i \sum_{k=1}^N z_k} e^{\frac{1}{2} \sum_{k=2}^N \sum_{l=1}^{k-1} [z_k, z_l]} \end{aligned} \tag{II.189}$$

Then from $[\hat{\pi}, \hat{\phi}] = i\hbar$ and with $\beta'_k := \beta_N - \beta_k$:

$$\frac{1}{\kappa_\phi \hbar} [z_k, z_l] = \langle \mathrm{ch}(c\beta'_l \omega) f_l, \frac{1}{\omega} \mathrm{sh}(c\beta'_k \omega) f_k \rangle_{L_2} - \langle \mathrm{ch}(c\beta'_k \omega) f_k, \frac{1}{\omega} \mathrm{sh}(c\beta'_l \omega) f_l \rangle_{L_2} \tag{II.190}$$

Now with

$$f_{\mathrm{ch}} := \sqrt{\frac{\hbar \kappa_\phi}{2\omega}} \sum_{k=1}^N \mathrm{ch}(c\beta'_k \omega) f_k, \qquad f_{\mathrm{sh}} := \sqrt{\frac{\hbar \kappa_\phi}{2\omega}} \sum_{k=1}^N \mathrm{sh}(c\beta'_k \omega) f_k \tag{II.191}$$

we see that (use finite time support of F (II.181))

$$\langle f_{\mathrm{ch}} - f_{\mathrm{sh}}, f_{\mathrm{ch}} + f_{\mathrm{sh}} \rangle_{L_2} = \frac{\hbar \kappa_\phi}{2} \sum_{k,l=1}^N \langle e^{-c\beta'_k \omega} f_k, \omega^{-1} e^{c\beta'_l \omega} f_l \rangle_{L_2} = \tag{II.192}$$

$$= \frac{\hbar \kappa_\phi}{2} \int_{\beta_1}^{\beta_N} ds ds' \, \langle e^{-c(\beta_N - s)\omega} F(s), \omega^{-1} e^{c(\beta_N - s')\omega} F(s') \rangle_{L_2} = \frac{\hbar \kappa_\phi}{2} \int_{\beta_1}^{\beta_N} ds ds' \, \langle \frac{e^{c(s-s')\omega}}{\omega} F(s), F(t) \rangle$$

Thus we compute the first exponent in (II.189) using (II.184)

$$\begin{aligned} e^{i \sum_{k=1}^N z_k} &= e^{i\hat{\phi}[\sqrt{\frac{2\omega}{\hbar \kappa_\phi}} f_{\mathrm{ch}}] + i\hat{\pi}[\sqrt{\frac{2\omega}{\hbar \kappa_\phi}} f_{\mathrm{sh}}]} = e^{i(\hat{a} + \hat{a}^\dagger)[f_{\mathrm{ch}}] + i(\hat{a} - \hat{a}^\dagger)[f_{\mathrm{sh}}]} = e^{i\hat{a}[f_{\mathrm{ch}} + f_{\mathrm{sh}}] + i\hat{a}^\dagger [f_{\mathrm{ch}} - f_{\mathrm{sh}}]} = \\ &= e^{i\hat{a}^\dagger [f_{\mathrm{ch}} - f_{\mathrm{sh}}]} e^{i\hat{a}[f_{\mathrm{ch}} + f_{\mathrm{sh}}]} e^{i[\hat{a}^\dagger [f_{\mathrm{ch}} - f_{\mathrm{sh}}], \hat{a}[f_{\mathrm{ch}} + f_{\mathrm{sh}}]]/2} = \\ &= e^{i\hat{a}^\dagger [f_{\mathrm{ch}} - f_{\mathrm{sh}}]} e^{i\hat{a}[f_{\mathrm{ch}} + f_{\mathrm{sh}}]} e^{\frac{\hbar \kappa_\phi}{4} \int_{\beta_1}^{\beta_N} ds ds' \langle F(s), \frac{e^{c(s-s')\omega}}{\omega} F(t) \rangle} \end{aligned} \tag{II.193}$$

giving the claimed result, when taking the vacuum expectation value.
And for the second with $\mathrm{sh}(a-b) = \mathrm{sh}(a)\mathrm{ch}(b) - \mathrm{ch}(a)\mathrm{sh}(b)$: (Note that $[z_k, z_k] = 0$)

$$\begin{aligned} \frac{1}{2} \sum_{k=2}^N \sum_{l=1}^{k-1} [z_k, z_l] &= \frac{\hbar \kappa_\phi}{2} \int_{\beta_1}^{\beta_N} ds \int_{\beta_1}^{s} ds' \, (\langle \mathrm{ch}(c(\beta_N - s')\omega) F(s'), \frac{1}{\omega} \mathrm{sh}(c(\beta_N - s)\omega) F(s) \rangle - \\ &\qquad - \langle \mathrm{ch}(c(\beta_N - s)\omega) F(s), \frac{1}{\omega} \mathrm{sh}(c(\beta_N - s')\omega) F(s') \rangle) = \\ &= \frac{\hbar \kappa_\phi}{2} \int_{\beta_1}^{\beta_N} ds \int_{\beta_1}^{s} ds' \langle \mathrm{sh}(c(\beta_N - s - \beta_N + s')\omega) F(s'), \frac{1}{\omega} F(s) \rangle = \\ &= -\frac{\hbar \kappa_\phi}{2} \int_{\beta_1}^{\beta_N} ds \int_{\beta_1}^{s} ds' \, \langle \mathrm{sh}(c(s-s')\omega) F(s), \frac{1}{\omega} F(s') \rangle_{L_2} \end{aligned} \tag{II.194}$$

where we used numerous times the self-adjointness of ω and that F is real-valued. □

We use the mentioned Lemma to evaluate the measure (II.182):

$$\begin{aligned}\mu(W[F]) &= \langle\Omega, e^{iz(f_N,\beta_N-\beta_N)}e^{iz(f_{N-1},\beta_N-\beta_{N-1})}...e^{iz(f_1,\beta_N-\beta_1)}\Omega\rangle_{\mathcal{H}} = \\ &= \exp\Big(\frac{\hbar\kappa_\phi}{4}\int dsds'\langle F(s), e^{c(s-s')\omega}\frac{1}{\omega}F(s')\rangle - \frac{\hbar\kappa_\phi}{2}\int_{s'\leq s} dsds'\langle \mathrm{sh}(c(s-s')\omega)F(s), \frac{1}{\omega}F(s')\rangle\Big) \\ &= \exp\Big(\frac{\hbar\kappa_\phi}{4}\int_{s'\geq s} dsds'\langle F(s), e^{c(s-s')\omega}\frac{1}{\omega}F(s')\rangle + \frac{\hbar\kappa_\phi}{4}\int_{s'\leq s} dsds'\langle F(s), e^{-c(s-s')\omega}\frac{1}{\omega}F(s')\rangle\Big) \\ &= \exp\Big(\frac{\hbar\kappa_\phi}{4}\int dsds'\langle F(s), e^{-c|s-s'|\omega}\frac{1}{\omega}F(s')\rangle_{L_2}\Big) \end{aligned} \tag{II.195}$$

It is worthwhile to note that this expression is indeed well-defined, as the operator $e^{\beta\omega}$ acting on all Schwarz functions F is only well-defined if $\beta < 0$.
Finally we will realise that

$$C := \frac{\hbar\kappa_\phi}{2}e^{-|x^0|\omega}\omega^{-1} = \hbar\kappa_\phi(-\partial^2/\partial(x^0)^2 + \omega^2)^{-1} \tag{II.196}$$

To see this we write the integral kernel of the latter:

$$((-\frac{\partial^2}{\partial(x^0)^2} + \omega^2)^{-1}F)(x) := \int d^{D+1}y\; G(x-y)F(y) \tag{II.197}$$

such that

$$(-\frac{\partial^2}{\partial(x^0)^2} + \omega_x)G(x-y) = \delta_{x,y} \tag{II.198}$$

This is solved by the Greens function

$$G(x) = \int \frac{d^{D+1}k}{(2\pi)^{D+1}}\frac{e^{ik_\mu x^\mu}}{k_0^2+\omega(k)^2} \tag{II.199}$$

with $\omega(k)^2 = \bar{k}^2 + p^2$ and using $\int dk \exp(ik(x-y)) = 2\pi\delta_{x,y}$. And indeed upon performing the k_0 integral via the residue theorem with the contours $\gamma_\pm$ being closed around the infinite half circle in the upper or lower complex plane respectively depending on the sign of x^0:

$$\int\frac{dk_0}{2\pi}\frac{e^{ik_0x^0}}{k_0^2+\omega(k)^2} = \int\frac{dk_0}{2\pi}\frac{e^{\pm ik_0|x^0|}}{k_0^2+\omega(k)^2} = \pm i\frac{e^{\pm i|x^0|(\pm i\omega(k)}}{\pm i\omega(k)2} = \frac{e^{-|x^0|\omega(k)}}{2\omega(k)} \tag{II.200}$$

and what remains is just the integral kernel of $e^{-|x^0|\omega}\omega^{-1}/2$ since

$$G(x-y) = \int\frac{dk^D}{(2\pi)^D}e^{i\bar{k}\cdot(\bar{x}-\bar{y})}\frac{e^{-|x^0|\omega(k)}}{2\omega(k)} = \frac{e^{-|x^0|\omega}}{2\omega}\delta_{\bar{x},\bar{y}} \tag{II.201}$$

So we find μ to be again a Gaussian measure, i.e.

$$\mu(W[F]) = \exp\left(\frac{\hbar\kappa_\phi}{2}\langle F, (-\partial_0^2+\omega^2)^{-1}F\rangle_{L_2(\mathbb{R}^{D+1})}\right) \tag{II.202}$$

II.D.3 Reconstructing the Canonical Formulation from the Measure

In the converse argument of the OS reconstruction we are given a measure μ which is reflection positive and invariant under time reflections and translations. Indeed, the measure (II.202) satisfies these criteria, which we show in the same way as [128]: Time translation and time reflection are obviously leaving the measure invariant, however for OS3 we need to do more work and consider the operator from the last line of (II.195), i.e. $e^{-c|s-s'|\omega}\omega^{-1}$ which describes the measure completely. We see for $F_t(x) := f(\bar{x})\delta_{t,x^0}$

$$\begin{aligned}\langle\theta F_t, (-\partial_0^2+\omega^2)F_t\rangle_{L_2(\mathbb{R}^{D+1})} &= \int dsds'\langle\theta F_t(s), e^{-c|s-s'|\omega}\frac{1}{\omega}F_t(s')\rangle = \\ &= \int dsds'\;\delta_{s,-t}\delta_{s',t'}\langle f, e^{-|s-s'|\omega}\frac{1}{\omega}f\rangle_{L_2} = \langle f, e^{-(t+t)\omega}\frac{1}{\omega}f\rangle_{L_2} \geq 0\end{aligned} \tag{II.203}$$

which extends due to Cauchy-Schwarz (II.12) to linear combinations thereof, i.e

$$F(t,x) := \sum_{k=1}^{N} \delta(t,t_k) f_k(x), \qquad G(t,x) := \sum_{l=1}^{M} \delta(t,s_l) g_l(x) \tag{II.204}$$

with $0 < t_1 < ... < t_N$, $0 < s_1 < ... < s_M$ and $f_k, g_l \in \mathcal{S}(\mathbb{R}^D)$. Thus on the history Hilbert space $V := L_2(\Gamma, d\mu)$

$$\begin{aligned}\langle e^{i\Phi[F]}, e^{i\Phi[G]} \rangle_V = \mu(e^{\Phi[G-\theta F]}) = e^{-\frac{1}{2}\langle G-\theta F, C(G-\theta F)\rangle_{L_2(\mathbb{R}^{D+1})}} = \\ = e^{-\frac{1}{2}\langle G, C\, G\rangle} e^{-\frac{1}{2}\langle F, C\, F\rangle} e^{\frac{1}{2}(\langle \theta F, C\, G\rangle + \langle G, C\theta\, F\rangle)}\end{aligned} \tag{II.205}$$

which can be used to show that the measure is indeed reflection positive. The proof for this is the following lemma from [135]:

Lemma II.D.2. *The Gaussian measure μ satisfies reflection positivity if C does.*

Beweis. We think of $a = \sum_J z_J e^{i\Phi[F_J]} \in V$ as an element $\sum_J z_J u_J$ in some Hilbert space U with basis $\{u_J\}_J$. Then a positive operator A on U is such that: $(z_J \in \mathbb{C})$

$$\sum_{IJ} z_I z_J A(u_I, u_J) \geq 0 \tag{II.206}$$

Then, on $U \otimes U$ the tensor product of two positive operators A, B is again positive: $(c_{IJ} \in \mathbb{C})$

$$\sum_{IJKL} c_{IJ} c_{KL} A(u_I, u_K) B(u_J, u_L) \geq 0 \tag{II.207}$$

(as can be seen by decomposing into eigenvectors of A, B respectively). But as the elements $\Psi = \sum_{IJ} z_I \delta_{IJ} u_I \otimes u_J \in U \otimes U$ generate a subspace of $U \otimes U$, $A \otimes B$ is still positive thereon. By iteration it follows that $N(.,.) = \exp(A(.,.))$ is positive.
Finally, since $\langle \theta ., C\, .\rangle$ is a positive form by (II.203), it follows that $\exp(\langle \theta ., C\, .\rangle)$ is also positive, which finishes the claim together with (II.205). □

Hence the necessary Osterwalder-Schrader axioms are satisfied.
According to Lemma II.C.1 we must determine the equivalence classes with respect to the Null space $\mathcal{N}$ of $\langle .,. \rangle_V$ in order to define the canonical Hilbert space $\mathcal{H}$. For this, we must at first understand the structure of V:

Lemma II.D.3. *The span of the vectors $e^{i\Phi[F]}$ with F of the form (II.204) lies dense in V.*

Proof. Let $H \in V = L_2(\Gamma, d\mu)$ of positive and compact time support in $(0, T]$ and consider

$$F^N(t) := \sum_{k=1}^{N-1} \delta(t, t_k) f_k^N(\bar{x}), \qquad f_k^N(\bar{x}) := \int_{t_k - T/(2N)}^{t_k + T/(2N)} dt\, H(t, \bar{x}) \tag{II.208}$$

with $t_k = kT/N$, $k = 1, ..., N-1$. It follows

$$||e^{i\Phi[H]} - e^{i\Phi[F^N]}||_V^2 = \mu(e^{i\Phi[H-\theta H]}) + \mu(e^{i\Phi[F^N - \theta F^N]}) - \mu(e^{i\Phi[H-\theta F^N]}) - \mu(e^{i\Phi[F^N - \theta H]}) \tag{II.209}$$

For instance the second term yields in the exponent

$$\langle F^N, C\, F^N \rangle_{L_2(\mathbb{R}^{D+1})} = \frac{\hbar \kappa_\phi}{2} \sum_{k,l=1}^{N-1} \langle F_k^N, e^{-c|t_k - t_l|\omega} \omega^{-1} F_l^N \rangle_{L_2} \tag{II.210}$$

which is just a Riemann sum approximation of $\langle H, C\, F\rangle_{L_2(\mathbb{R}^{D+1})}$. The other calculations are similar and show that

$$||e^{i\Phi[H]} - e^{i\Phi[F^N]}||_V^2 \underset{N\to\infty}{\longrightarrow} 0 \tag{II.211}$$

And we have already seen that by linear combinations and functional derivative any vector can be constructed from the $e^{i\Phi[H]}$. Hence the span of these vectors is dense in V. □

Now we will show that the equivalence classes with respect to $\mathcal{N}$ are exactly given by functions of time zero support. Indeed for any G of positive sharp time support as in (II.204) we define the time zero function

$$G^0(t,\bar{x}) := \delta(t,0)(\sum_l e^{-cs_l\omega} g_l)(\bar{x}) \tag{II.212}$$

Then follows from

$$\begin{aligned}\langle \theta F, C\, G\rangle_{L_2(\mathbb{R}^{D+1})} &= \langle F, C\theta G\rangle_{L_2(\mathbb{R}^{D+1})} = \frac{\hbar\kappa_\phi}{2}\int dsds'\ \langle e^{-c|s-s'|\omega}F(s), \omega^{-1}G(-s')\rangle_{L_2} = \\ &= \frac{\hbar\kappa_\phi}{2}\int dsds'\ \langle e^{-(s+s')\omega}F(s), \omega^{-1}G(s')\rangle_{L_2} = \\ &= \frac{\hbar\kappa_\phi}{2}\sum_{k,l}\langle e^{-ct_k\omega}f_k, \omega^{-1}e^{-cs_l\omega}g_l\rangle_{L_2} = \langle \theta F, C\, G^0\rangle_{L_2(\mathbb{R}^{D+1})}\end{aligned} \tag{II.213}$$

that for all F (using (II.205))

$$\langle e^{i\Phi[F]}, e^{i\Phi[G]} - z e^{i\Phi[G^0]}\rangle_V = 0 \tag{II.214}$$

with $z := \exp(-\frac{1}{2}(\langle G, C\, G\rangle_{L_2(\mathbb{R}^{D+1})} - \langle G^0, C\, G^0\rangle_{L_2(\mathbb{R}^{D+1})}))$. Thus we conclude that any vector of positive time support can be approximated by the $e^{i\Phi[H]}$, $H \in \mathcal{S}(\mathbb{R}^{D+1})$ of positive time support. By Lemma II.D.3 this allows to approximate it instead by the $e^{i\Phi[F]}$ with F of sharp time support, which due to the last computation (II.214) is equivalent to vectors of time zero support. Hence $\mathcal{H}$ is the completion of the span of vectors of sharp time zero support $F^0 = \delta(t,0)f$, for which we have by (II.195)

$$\langle e^{i\Phi[F^0]}, e^{i\Phi[F'^0]}\rangle_{\mathcal{H}'} = e^{-\frac{\hbar\kappa_\phi}{4}\langle f,\omega^{-1}f\rangle_{L_2}} = \langle e^{i\hat{\phi}[f]}, e^{i\hat{\phi}[f']}\rangle_{\mathcal{H}} \tag{II.215}$$

displaying $\mathcal{H} = L_2(\mathcal{S}(\mathbb{R}^D), d\nu)$ where ν is a Gaussian measure. Here $e^{i\hat{\phi}[f]} := [e^{i\Phi[F^0]}]$ denotes the equivalence class of the sharp time zero support vector.
Following the OS reconstruction we set $\Omega := 1 = [1]$ and determine the Hamiltonian $\hat{H}$ via the finite time translations: (use (II.214) for the second line)

$$\langle e^{i\hat{\phi}[f]}, e^{-\beta\hat{H}/\hbar} e^{i\hat{\phi}[f']}\rangle_{\mathcal{H}} := \langle e^{i\Phi[F^0]}, R\, e^{i\Phi[T_{-\beta}F'^0]}\rangle_{\mathcal{E}} = \mu(e^{i\Phi[T_\beta F'^0 - F^0]}) = \tag{II.216}$$

$$= \mu(e^{i\Phi[(e^{-c\beta\omega}f' - f)\delta_{t,0}]}) = e^{-\frac{1}{2}(\langle T_\beta F'^0, CT_\beta F'^0\rangle - \langle e^{-c\beta\omega}f'\delta_{0,.}, Ce^{-c\beta\omega}f'\delta_{0,.}\rangle)}\langle e^{i\hat{\phi}[f]}, e^{\hat{\phi}[e^{-c\beta\omega}f']}\rangle_{\mathcal{H}} \tag{II.217}$$

And as the span of $\hat{w}[f]\Omega := \exp[i\hat{\phi}[f]\Omega$ is dense in $\mathcal{H}$ it follows:

$$e^{-\beta\hat{H}/\hbar}\hat{w}[f]\Omega = e^{-\frac{\hbar\kappa_\phi}{4}(\langle f,\omega^{-1}f\rangle - \langle e^{-\beta c\omega}f, \omega^{-1}e^{-\beta c\omega}f\rangle)}\hat{w}[e^{-\beta c\omega}]\Omega \tag{II.218}$$

which we find to be in correspondence with (II.180).

Kapitel III

Renormalisation

Although the last chapter presented all the necessary tools for developing a quantum field theory (QFT), as of today no interacting QFT in four spacetime dimensions has been constructed so far that satisfies the Wightman axioms. Instead, many experiments could be described with high precision using perturbation theory. However, in general very little is known about the convergence of the perturbation series. To make matters worse, we found a lot of ambiguities arising during quantisation. In the canonical formulation, the ambiguities were 1) the non-commutative $\star$-product and the sub set $\mathcal{E}$ on which it is implemented and 2) its representation $(\pi, \mathcal{H}, \Omega)$ or, in other words, the state ω. These are mutually independent choices and, in the context of a field theory, they are all non-trivial.
In this regard, the situation improves slightly when we investigate systems with finitely many degrees of freedom. This is typically the case in mechanics where a classical D-dimensional particle can be described by $2D$ numbers, i.e. its position in coordinate space q and its momentum p. (In contrast to this, a field will have arbitrary values at any point in space, of which there are uncountably many.) The choice of the state ω on the quantum algebra becomes very simple, if we restrict our attention to the subclass of states, which are *regular* and whose GNS representation is irreducible. This means that their *Weyl elements* $w[x,y](q,p) = \exp(i(y\hat{q}+x\hat{p})/\hbar) \in C^\infty(\mathcal{F})$ are strongly continuous. Indeed, due to the famous *Stone-von Neumann theorem* [192–195], every such representation is equivalent to a single one, namely the Schrödinger representation $(\pi_S, L_2(\mathbb{R}, dx))$. This is the representation of the *Fock state* ω^l which reads for one particle in one dimension:

$$\omega^l \; (\; w[x,y] \;) \; = \; \exp\,(-\frac{1}{4}(\frac{x^2}{l^2} + \frac{y^2 l^2}{\hbar^2})\,) \tag{III.1}$$

where $l > 0$. This mathematical proof tells us that, for any representation $(\pi^j, \mathcal{H}^j)$ we consider, there is a unitary map $U_j : \mathcal{H}^j \to L_2(\mathbb{R}, dx)$ such that for all $a \in \mathcal{A}$ we have $\pi_S(a) = U_j \pi(a) U_j^\dagger$. This simplifies the situation drastically as it not only provides a uniqueness result, but moreover tells us how to find straightforwardly the corresponding quantum theory, whose predictions can then be put to the test. However, the crucial condition for this theorem to work is that the system under consideration has finitely many degrees of freedom and is regular in its Weyl elements.[1]

Hence, it is not applicable to a field theory which carries infinitely many degrees of freedom on a continuous manifold. However, a possible alternative, due to which we can maybe hope to use this theorem (at least in some cases) again, comes from the following line of thoughts: The infinitely many degrees of freedom come from points in space which have arbitrary close neighbours, yet it is clear that this might be information to which we - as humans - do not have access: Our measurement apparatus will always be far from perfect and we do not expect to measure a field directly at a point in space. Instead, we are normally able to detect what the mean value of the field over a certain region is. Consider different ways to split our spatial manifold into disjoint unions of small regions B_ϵ where ϵ serves as a parameter to label those discretisations.[2] For each region B_ϵ we associate a characteristic function χ_ϵ, which is vanishing everywhere outside of B_ϵ and constant inside. We assume that, through our experiment, we will detect $\phi[\chi_\epsilon], \pi[\chi'_\epsilon] \in \mathbb{C}$, in other words with each region χ_ϵ we can associate an observable, e.g. the spatial Weyl elements $w[\chi_\epsilon, \chi'_\epsilon] = \exp(i(\phi[\chi_\epsilon] + i\pi[\chi'_\epsilon])) \in C^\infty(\mathcal{F})$ for the field value and its momentum dependent analogues. If we would choose as the subalgebra of observables

[1] We will later encounter a system of finitely many degrees of freedom, for which the Weyl elements are indeed not strongly continuous. This particular example is a proposal for a quantum theory of cosmology and called *Loop Quantum Cosmology*.

[2] We will demand that ϵ is valued in some partially ordered index set, where $\epsilon > \epsilon' \Leftrightarrow$ for all $B_{\epsilon'}$ we find some B_ϵ such that $B_{\epsilon'} \subset B_\epsilon$.

$\mathcal{A}$ the span of these functions for a finite set of regions which parcel our (compactified[3]) manifold, then we call this the *discretisation* of the continuum algebra labelled by the discretisation parameter ϵ. Here, we associate $\epsilon \to 0$ with increasingly better resolution. It might be tempting to think about this set of *discrete* functions as the basic variables of a new system with finitely many degrees of freedom, that we could hope to quantise along the lines of the Stone-von Neumann theorem. The idea would be to choose as algebra the span of block functions, i.e. $a \in \mathcal{A}_\epsilon$ implies $a = \sum_{nm} c_{nm} w[\chi_{n,\epsilon}, \chi_{m,\epsilon}]$ for some choice $\chi_{n,\epsilon}$ where n is a label for all regions B_ϵ at a fixed resolution ϵ. Then we could write any state (if some exist) which is regular in those Weyl elements as a direct product of Fock states ω^l for each block. However, we *must not* forget about time evolution and have to determine the expectation value $\omega_\epsilon(H)$ for the Hamiltonian H. Yet this is typically not a function of the field at this coarse resolution. In other words, it cannot be written as $H'(\{w[\chi_\epsilon, \chi'_\epsilon]\})$ and hence its action is not a priori defined in this Hilbert space.
However, it might not even be necessary to consider the full Hamiltonian: since we are only able to measure the mean value of the field on some regions B_ϵ, all that we want our theory to predict is how these values change over time given some initial data. So instead of the Hamiltonian H we are interested in a map from coarse resolution onto itself that agrees with the predictions from the Hamiltonian. We will call this map the discretised Hamiltonian H_ϵ. Indeed, it is a whole family of Hamiltonians, one for each label ϵ, and it is a priori not clear how they are built as functions $H_\epsilon(\{w[\chi_\epsilon, \chi'_\epsilon]\}, \epsilon)$, knowing only their continuum origin H.
A (necessary but not sufficient) idea as a criterion to determine H_ϵ for a given theory is to consider a very small discretisation ϵ. If the parcellation B_ϵ of our manifold is sufficiently small, then every continuous field ϕ can be well approximated by stair-case functions $\phi_{\mathrm{App},\epsilon}$ over the χ_ϵ, up to mistakes of order ϵ and similar for its momentum. In other words, for $\epsilon \to 0$ we find better and better approximations, such that the error vanishes in the end. In the same spirit, we could hence approximate the Hamiltonian $H \approx H_{\mathrm{App},\epsilon}$, which is a functional over the field, up to some error in ϵ. Choosing this approximation for our discretised family $H_\epsilon := H_{\mathrm{App},\epsilon}$ would guarantee us that, in the so called *continuum limit* $\epsilon \to 0$, we are to obtain the original theory. However, as we said, this criterion does not yet automatically determine the correct discretised Hamiltonian as, by the same logic, we could also choose $H_\epsilon := H_{\mathrm{App},\epsilon} + \epsilon f$ for any function f such that $\epsilon f \to 0$ for $\epsilon \to 0$. Thus, this *criterion of the continuum limit* has introduced a whole new range of possible choices for the quantum Hamiltonian, i.e. *quantisation ambiguities*![4]

It seems that this procedure has only transferred the ambiguities from 2) to a new set of ambiguities and there would have been no gain. However, this is not the case as the criterion for the continuum limit is a necessary but by far not a sufficient condition for determining the discrete Hamiltonian H_ϵ. The main feature is that all H_ϵ are restrictions of the continuum Hamiltonian to the discrete observables. However, their action on the coarse observables is supposed to be exactly the same as the continuum Hamiltonian at *any* resolution. This is a far stronger demand than that the family H_ϵ should agree in its continuum limit. Hence it is expected to bring new insight. It is known in the literature as *cylindrical consistency condition* and it tells us the following: If we have a field whose information can be fully grasped at coarse resolution 2ϵ, then a finer resolution ϵ will of course not contain any new insight. The physical predictions, when looking at an observable at resolution ϵ or 2ϵ, do not change, i.e.

$$\omega_{2\epsilon}(\, w[\chi_{2\epsilon}]\,) \;=\; \omega_\epsilon(\, w[I_{2\epsilon\to\epsilon}\chi_{2\epsilon}]\,) \tag{III.2}$$

where the *injection map* $I_{2\epsilon\to\epsilon}$ is telling us that we should regard the block $B_{2\epsilon}$ as composed of its smaller sub blocks at resolution ϵ with respect to which ω_ϵ is defined. This must be true for any observable and especially for the family of Hamiltonians H^ϵ. Once the Hamiltonian is chosen on a given resolution as a fixed function $H(\chi_\epsilon, \epsilon)$, then, via (III.2), we can determine the corresponding function $H'(\chi_{2\epsilon}, 2\epsilon)$ at any other coarser resolution.
Note, however, that $H'(..., \epsilon)$ might in general be different from $H(..., 2\epsilon)$, in other words, the physical predictions of the theory depend on the resolution with respect to which an experiment takes place. For this *not* to be the case, our family H_ϵ must not change under the cylindrical consistency condition $H_\epsilon \to H_{2\epsilon}$ implied by (III.2). Hence, it must be a *fixed point* of this map.
In total: the discrete projections of a continuum theory can be uniquely quantised (up to the choices 1)) by picking as Hamiltonian a cylindrically consistent fixed point!

[3] In order to get a finite set of observables, we have indeed to consider compact manifolds. In case $\mathcal{M}$ is not compact, we will hence introduce infrared cut-offs: a spatial one called R and a temporal one called T. After having constructed our QFT, these will be removed in the statistical physics sense. Note hence that, in the following, everything depends in principle on the parameters T and R.

[4] That these ambiguities indeed carry non-trivial consequences will be demonstrated in the last chapter of this thesis *V. Loop Quantum Gravity*. We study the differences in predictions arising for chosen discretisations of the Hamiltonian in the field theory GR (which we introduce in the next chapter).

As our task of defining an interactive quantum field theory is crucially dependent on finding a non-trivial fixed point, we will invoke a procedure by which one can hope to find this fixed point: the *renormalisation group*.
Although we have been talking so far only about the canonical point of view, the renormalisation group (RG) was originally designed for applications in the context of covariant quantisation. Inspired by the seminal paper from Gell-Mann and Low [100] and the block-spin transformations by Kadanoff [101], it was developed by Wilson and Kogut [102–105] and later extended by many others [106–114]. However, while stemming from the same philosophy, the technical implementation was quite different as one had to deal with defining a spacetime path integral formalism. The details of this approach will be outlined in *III.A. Standard Renormalisation*. Indeed, the rigorous definition of the path integral in the presence of finitely many degrees of freedom is possible even for interacting theories, at least while on Minkowski space. The starting point of the renormalisation programme is an (arbitrary) naive discretisation family of spacetime measures $N, M \to \mu^{(0)}_{N,M}$ which only satisfy the continuum limit condition (Here, $M = \frac{1}{\epsilon}$ refers to a spatial UV cut-off, whereas N is the inverse of some temporal UV cut-off). We will choose the same ad hoc prescription at all spatial and temporal resolutions N, M. Then, we define the history fields $\Phi_{N,M}$ at discrete resolution simply as the continuum history field smeared with test function of the same coarse resolution, i.e. $\Phi_{N,M}[F] := \Phi[F]$. The coarse functions F are of a special kind, namely: for each resolution N, M we consider a set of finitely many numbers $F_{N,M}(n,m) \in \mathbb{R}$, one for each region $B_{n,m}$ of the parcellation of $\mathcal{M}$. The space of all $F_{N,M}$ is called $L_{N,M}$. Then, a function of coarse resolution N, M is exactly $F = I_{N,M} F_{N,M} := \sum_{n,m} \chi_{n,m}(x,t) F_{N,M}(n,m)$, in other words, on region $B_{n,m}$ the function has the constant value $F_{N,M}(n,m)$. The map $I_{N,M}$ which associates the set of numbers with a function in the continuum is called *injection map*. Now, knowing the measure of a distinct element in the spacetime configuration space, i.e. the time dependent Weyl element $W[F_{N,M}]$ with $W_{N,M}[F_{N,M}](\Phi) := \exp(i\Phi_{N,M}[F_{N,M}])$ gives us full control as every other observable can be constructed by suitable linear combinations and derivatives. From this initial family of measures $\mu^{(0)}_{N,M}$, we will now construct a sequence of measure families $\mu^{(n)}_{N,M}$, where each element is obtained from the previous one by integrating out the degrees of freedom at resolution $M/2$ and $N/2$ that do not contribute to resolution N, M. If this series converges to a point in the space of all possible measures, this measure, called $\mu^{*}_{N,M}$, will automatically satisfies the spacetime version of the cylindrical consistency condition, namely

$$\mu_{N,M}(W_{N,M}[F_{N,M}]) = \mu(W[I_{N,M}F_{N,M}]) = \mu_{2^n N, 2^m M}(W_{2^n N, 2^m M}[I_{N,M \to 2^n N, 2^m M} F_{N,M}]) \,. \qquad \text{(III.3)}$$

where the *injection map* $I_{N,M \to 2N,2M}$ is telling us that we should regard any block of resolution N, M as composed of its smaller sub blocks at resolution $2N, 2M$ with respect to which $\mu_{2n,2M}$ is defined.

While well understood and having a huge success in the field of covariant quantum theory, the canonical side of the renormalisation group has been largely undeveloped. Thus, we try to develop a background independent version of it in the canonical context as derived in the papers [128–131]. First, let us emphasise that we will not use the Fock state indicated above for our initial discretisation: Assuming we are given an initial guess for a Hamiltonian $\hat{H}^{(0)}_M$, we will consider the vacuum vector $\Omega^{(0)}_M$ annihilated by the Hamiltonian and choose it to build the state for the corresponding vacuum expectation values. However, in this framework, we do not just have to renormalise and search for the fixed point of the Hamiltonian sequence $H^{(n)}_M$, but also for the fixed points of the associated vacuum vector sequence $\Omega^{(n)}_M$ and the generated Hilbert spaces $\mathcal{H}^{(n)}_M$.
The reason for this is rooted in the fact that in this language we have an easier transition to the results obtained in chapter *II. Quantum Field Theory*. There, we were able to show that there is a bijection between these so-called OS data, which describe completely a canonical theory, and a subset of all possible spacetime measures, namely those which are satisfying (a subset of) the Osterwalder-Schrader axioms. Hence, by adapting our formulation to this description, we can revert to the way the RG is treated in the covariant setting.

This motivates us to try to close the following diagram, figure III.1. We want to develop a framework of Hamiltonian renormalisation in such a way that we determine a flow for the sequences of the triple $(\mathcal{H}^{(n)}_M, \hat{H}^{(n)}_M, \Omega^{(n)}_M)$ which leads to the same fixed point we would have obtained after Osterwalder-Schrader reconstruction of the fixed point of the spacetime measure sequence $\mu^{(n)}_M$. Indeed, it will turn out that the discretisation of a measure obtained from OS construction is already a fixed point of temporal renormalisation and hence we will drop the label N. Although this means that we must renormalise three quantities instead of one, the task will be much simplified as it is easier to study the flow of these objects instead of a flow on the space of path integral measures.
As it turns out, one will only be partially successful with this strategy: As the OS reconstruction demands that the elements of the obtained Hilbert space are equivalence classes with respect to the null space of

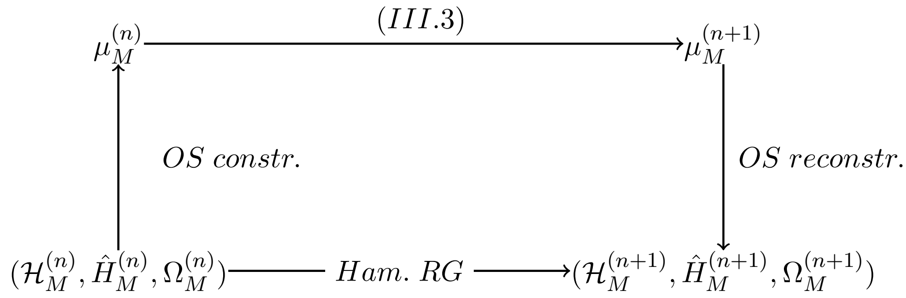

Abbildung III.1: The path-integral induced Hamiltonian renormalisation group is developed such that its fixed point theory *must* agree with the fixed point covariant measure.

the measure, it is essential to construct it! Of course, this is contrary to the original purpose of simplifying the task of renormalisation. Yet, it is a procedure by which a cylindrically consistent quantum theory can be obtained. Hence, we will give a brief overview over the *path-integral induced Hamiltonian renormalisation*:

1. Pick an initial discretisation family $(\mathcal{H}_M^{(0)}, \hat{H}_M^{(0)}, \Omega_M^{(0)})$, labelled by M. Determine the history space measure $\mu_M^{(0)}$ via OS construction.

2. Determine the family $\mu_M^{(n+1)}$ via
$$\mu_M^{(n+1)}(W_M[F_M]) := \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}F_M]) \ . \tag{III.4}$$
Use this to define the equivalence class $[.]_{\mu_M^{(n+1)}}$ of the OS reconstruction and give rise to a map $J_{M\to 2M}^{(n)}$ such that it embeds $\mathcal{H}_M^{(n+1)}$ into $\mathcal{H}_{2M}^{(n)}$.

3. Set $\Omega_M^{(n+1)} = [1]_{\mu_M^{(n+1)}} = (J_{M\to 2M}^{(n)})^\dagger \Omega_{2M}^{(n)}$. Let $\mathcal{H}_M^{(n)}$ be the span of the $[W_M[F_M]]_{\mu_M^{(n+1)}}$. Determine $\langle .,.\rangle_{\mathcal{H}_M^{(n)}}$ or equivalently the Hilbert space measure $d\nu_M^{(n)}$ by demanding that $J_{M\to 2M}^{(n)}$ is an isometry. Set
$$\hat{H}_M^{(n+1)} := (J_{M\to 2M}^{(n)})^\dagger \hat{H}_{2M}^{(n)} J_{M\to 2M}^{(n)} \ . \tag{III.5}$$

4. Start over at step 2 until you run into a fixed point $(\mathcal{H}_M^*, \hat{H}_M^*, \Omega_M^*)$ and μ_M^* for $n\to\infty$.

But, as this procedure demands the construction of the history-space measure μ_M^*, it is not worthwhile to use it: instead, one would simply perform an OS reconstruction at the end after having performed just the renormalisation of the history-space measure (which has to be carried out anyway). Thus, we will propose an alternative route of renormalisation in *III.B. Hamiltonian Renormalisation*, which is called *direct Hamiltonian renormalisation* in [128]. The philosophy behind this incarnation is as follows: Originally, we wanted to study the continuum QFT. But although we were not able to construct the state ω explicitly, we *assume* that such a continuum Hilbert space $\mathcal{H}$ equipped with continuum Hamiltonian $\hat{H}$ exists. Then, all Hilbert spaces of discrete resolution $\mathcal{H}_M$ should be embeddable in this continuum Hilbert space, via some resolution-dependent isometric embedding map j_M. Any operator, defined on $\mathcal{H}$, is then also defined on the sub space, which is the image of any j_M. E.g., for the Hamiltonian $\hat{H}$ in $\mathcal{H}$, this motivates to define on $\mathcal{H}_M$:
$$\hat{H}_M^* \ := \ j_M^\dagger \ \hat{H} \ j_M \ . \tag{III.6}$$
To compare vectors in two Hilbert space of different resolution M, M', we could use $j_M, j_{M'}$ to embed both into $\mathcal{H}$. This motivates to consider the concatenation $j_{M\to M'} := j_{M'}^\dagger \circ j_M$, called the "coarse graining map". It offers itself, to choose a M' as refinement of M, for example on a cubic lattice $M < M' = 2M$. This motivates the following (improved) renormalisation procedure:

1. Pick an initial discretisation family $(\mathcal{H}_M^{(0)}, \hat{H}_M^{(0)}, \Omega_M^{(0)})$, labelled by M, where $\mathcal{H}_M^{(0)}$ is spanned by $\pi(w_M[f_M])\Omega_M^{(0)}$ for different $f_M \in L_M$.

2. Set $\Omega_M^{(n+1)} = (j_{M\to 2M}^{(n)})^\dagger \Omega_{2M}^{(n)}$. Set $\mathcal{H}_M^{(n+1)} = span\{\pi(w_{2M}[I_{M\to 2M}f_M])\Omega_M^{(n)};\ f_M \in L_M\}$. Demand the embedding j_M to be isometric, which is equivalent to
$$\nu_M^{(n+1)}(w_M[f_M]) := \nu_{2M}^{(n)}(w_{2M}[I_{M\to 2M}f_M]) \tag{III.7}$$

and for the Hamiltonian

$$\hat{H}_M^{(n+1)} = (j_{M\to 2M}^{(n)})^\dagger \hat{H}_{2M}^{(n)} j_{M\to 2M}^{(n)} \, . \tag{III.8}$$

3. Start over at step 2 until you run into a fixed point $(\mathcal{H}_M^*, \hat{H}_M^*, \Omega_M^*)$ for $n \to \infty$.

The advantage of the latter scheme is that the direct Hamiltonian renormalisation is better executable as it sidesteps the necessity to renormalise the spacetime measure at each step. However, it remains to be confirmed that this modified scheme results in physically viable fixed points as the original path-integral induced Hamiltonian renormalisation did.

Having now defined the toolbox by which we hope to find a cylindrically consistent theory, we shall test it in the simplest example over which we have full control: the free Klein Gordon scalar field.
In section *III.C. Example: Klein Gordon field I - Derivation*, we will use both schemes to determine the fixed point in one spatial dimension. It turns out in [129] that one can determine its analytical structure explicitly as the initial Hilbert space measure suggests itself to be picked as a Gaussian measure, a property which will be preserved in each renormalisation step. Hence, we find

$$\nu_M^*(\, w[f_M]\,) \;=\; \exp(\, -\frac{\hbar\kappa_\phi}{4}\, \langle f_M, C_M^* f_M\rangle_M \,) \tag{III.9}$$

with an involved fixed point *covariance* matrix C_M^*. It is interesting to note that both schemes differ drastically already after the first renormalisation step as the path-integral induced Hamiltonian renormalisation develops a dependence on infinitely many independent field species at the finite resolution M. These contributions appear due to the necessity to deal with the equivalence classes of the spacetime measure. However, all but one field species will develop an infinite mass in the continuum limit and vanish again. This demonstrates that at least for free QFT the direct Hamiltonian renormalisation makes more immediate contact to the projections of the continuum theory than the path-integral induced Hamiltonian renormalisation does, albeit resulting in the same continuum theory. This motivates to study the direct Hamiltonian renormalisation further, although it remains to be seen whether this continues to hold in the case of interacting theories. This is an important question for further studies.

But there remain a lot of open questions regarding this procedure. While we have only constructed the fixed point as it stands, we have not shown that the procedure, as advocated above, really works. To be concrete, in the previous section, we merely found the fixed point by close investigation, not by iterating the flow $n \to \infty$. As, in more general situations, it might not be possible to circumvent this step, we will present a more thorough investigation of the flow in section *III.D. Example: Klein Gordon field II - Properties*.
Afterwards, we must remember that there were still arbitrary choices during the renormalisation procedure. For one, the choice of the coarse graining map is only restricted by a few conditions, e.g. it must be cylindrically consistent. Moreover, several different initial discretisations could have been chosen in the beginning. We restrict the possible choices by demanding that the naive continuum limit of the classical Hamiltonian $H_M^{(0)}$ shall reduce to the continuum Hamiltonian function. As the renormalisation procedure is supposed to only introduce corrections of order of the lattice spacing, i.e. $\mathcal{O}(\epsilon)$, we hope that the property to give the correct continuum limit is being kept at all iterations. However, this criterion is far from sufficient, as we have already discussed: There are a lot of quantisation ambiguities and it is not clear whether they might all lead to different cylindrically consistent fixed points if we investigate a given cylindrically consistent flow of these starting points. If there exists a unique fixed point for all discretisations, then we refer to it as *universal*. To the best of our knowledge, the universality property, in this sense, is not well understood for general theories. However, in [130] we discussed that, for the free field, the fixed point described by (III.9) is obtained in the limit $n \to \infty$ for a whole class of possible discretisations and is hence at least partly subject to the universality feature.
But, nonetheless, it is highly dependent on the choice of injection map $j_{M\to 2M}$ which we will also discuss. In the literature, there exist, moreover, different renormalisation group schemes not implementing cylindrical consistency, which are not suitable for our purposes.

Lastly, we will extend the computations from above to the case of arbitrary spatial dimensions in *III.E. Example: Klein Gordon field III - Rotational Invariance*. As the title already suggests, this extension enables us to study the restoration of continuum properties such as rotational invariance.
In [131] the injection map $I_{M\to 2M}$ in several dimensions was chosen to be the product of injection maps for each spatial direction separately. Then, the techniques developed for one spatial dimension can be transferred

to any number of spatial dimensions D. To illustrate this, we work out the case of $D = 2$ explicitly.
The continuum Klein Gordon field, described by covariance C, is a theory which is rotationally invariant, i.e. for the representation Π of the rotation group on the finite spatial torus we have, for all angles $\alpha \in [0, 2\pi)$,

$$\langle f,\ C\ f' \rangle \ =\ \langle\ \Pi(\alpha) f,\ C\ \Pi(\alpha) f'\ \rangle \tag{III.10}$$

for all functions f, f' which are time independent. A natural question to study is how such a symmetry transfers to coarse projections on a lattice which itself is not rotationally invariant. However, by considering the whole family of discretisations at all resolutions M, a peculiar feature occurs: first, we consider the realisation from [212, 213] that every rotation can be arbitrarily well approximated by successively rotating several times around a single angle θ, given $\theta/(2\pi)$ is irrational. For example, one can choose $\cos(\theta) = 3/5$ and rotational invariance is obtained once invariance for rotations by θ is shown. The second observation is that a lattice at resolution M, rotated by the aforementioned choice for θ can be completely embedded in its unrotated refinement at resolution $5M$. This allows us to approximate $C_{\theta M}$, the covariance of the rotated lattice, completely by C_{5M}, the covariance at finer resolution. The condition for *rotational invariance* of the fixed point can then be written in terms of its Fourier transform as

$$\hat{c}^*_M \ \stackrel{!}{=}\ \hat{c}^*_{\theta M} \ +\ \mathcal{O}(\epsilon^5) \ =\ P(\hat{c}^*_{5M}) \ +\ \mathcal{O}(\epsilon^5) \tag{III.11}$$

where c_M is the rescaled, unit-free C_M and P is an involved, but explicit function. And indeed, this criterion will be met when investigated with numerical methods. This indicates the restoration of continuum symmetries even at the coarse resolutions, which gets increasingly better as the resolution becomes finer, see figure III.2.

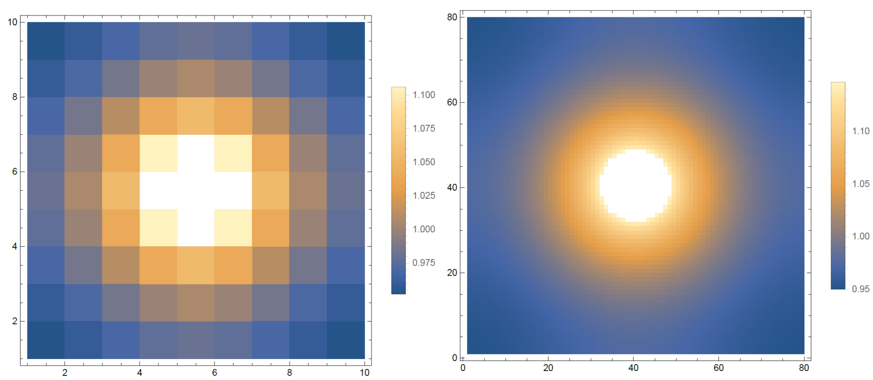

Abbildung III.2: The rescaled fixed point covariance c^*_M as obtained by the direct Hamiltonian renormalisation procedure in $D = 2$. The matrix element is translation invariant $c^*_M(m, m') = c^*_M(m - m')$, $m \in \mathbb{Z}^2_M$, and plotted from $m - m' \in [-M/2, M/2]^2$ with centre point $m = (0, 0)$ in the middle of both pictures. The values on the corners agree with each other, due to the periodic boundary conditions, and represent the covariance for maximally separated points. Blue colours indicate small numerical values, while orange colour indicates higher values. Due to the exponential increase towards the middle, the values of the points closest to $(0, 0)$ lie above of the plotted range and are depicted in white. The covariances for resolution $M = 10$ (left) and for $M = 80$ (right) show an improvement of rotational invariance for higher resolutions.

This finishes a complete analysis of the Klein Gordon field and justifies the method of direct Hamiltonian renormalisation. Hence the stage is set to apply it in a more difficult context, e.g. Quantum Gravity.
In the remainder of this chapter, we now quote the calculations of the papers [128–131] and supplement them by further thoughts.

III.A Standard Renormalisation

In this section we review the renormalisation approach as it was originally pioneered by Gell-Mann and Low [100] and Kadanoff [101]. The formulation here is mainly the one designed in the seminal papers by Wilson and Kogut [102–104]. It is manifestly designed for the covariant approach and hence called the *path integral renormalisation group* method. Although it is well documented in the literature, we will review the main ingredients for completeness and to introduce language adaptations from [128] that will be used in the remainder of this chapter.
We base our work on a triangulation of a manifold $\mathcal{M} \cong \mathbb{R} \times \sigma$ with $\sigma = \mathbb{R}^D$ equipped with flat Minkowski

metric $\eta_{\mu\nu}$.[5] Then it is logical to consider a regular discretisation, e.g. a hypercubic lattice, with distinct lattice spacings for time and space direction. Although they are often considered to be the same, we will carefully distinguish between the two, as it is our aim in the subsequent sections to achieve the transition to a Hamiltonian version of renormalisation, wherein time will be continuous and hence fundamentally different from the still discretised space. Thus, in the following we choose an infrared (IR) spatial cut-off $R \in \mathbb{R}_+$ and an IR temporal cut-off $T \in \mathbb{R}_+$. In other words, we consider the compactified manifold $\mathcal{M} \to \mathcal{M}_{T,R} \cong [0,T) \times \sigma_R$ with $\sigma_R \cong [0,R]^D$. On the compactified manifold we introduce the ultraviolet (UV) cut-offs ϵ (spatial) and δ (temporal).

III.A.1 Construction of coarse Observables from the Continuum

Instead of dealing with test functions F on $\mathcal{M}$ we are now much more interested in functions supported on the finally many points of $\mathcal{M}_{T,R}$ which are labelled by the parameters R, ϵ, T, δ. Indeed, there are $M = R/\epsilon$ many lattice cells in each spatial direction and $N = T/\delta$ many cells in temporal direction. We will thus adopt the following notation: $L_{N,M} := \ell_2(\mathbb{Z}_N \times \mathbb{Z}_M^D)$ is the space of all functions $F_{N,M} : \mathbb{Z}_N \times \mathbb{Z}_M^D \to \mathbb{R}$ with $\mathbb{Z}_M := \{0, 1, ...M-1\}$; $L_{T,R} := L_2([0,T) \times [0,R)^D, d^{D+1}x)$ is the space of all square-integrable functions $F : \mathcal{M}_{T,R} \to \mathbb{R}$; lastly $L := L_2(\mathcal{M}, d^{D+1}x)$ is the space of all square-integrable functions $F_c : \mathcal{M} \to \mathbb{R}$.
We will understand the transition from $\mathcal{M}_{T,R}$ to $\mathcal{M}$ in terms of a thermodynamical limit and are hence foremost interested in the relation between the truncated lattice space $\mathbb{Z}_N \times \mathbb{Z}_M^D$ and $\mathcal{M}_{T,R}$. To understand this relation, we must *postulate* a way by which physical quantities like the Weyl elements $W[F](\Phi)$, which are supported on $\mathcal{M}_{T,R}$ and on the space of which the final measure μ will be a functional, can be thought of as quantities on the lattice. The first step for this will be to relate test functions $F_{N,M}$ on the lattice with a certain subset of functions F on $\mathcal{M}_{T,R}$, which we will refer to in the following as *embedding* $L_{N,M}$ into $L_{T,R}$:

Definition III.A.1 (Evaluation & Injection maps for scalar fields). *In case of a scalar field theory we consider the discretised fields:*

$$\Phi_{N,M}(n,m) := \Phi[\chi_{n\delta,m\epsilon}] \tag{III.12}$$

We call the evaluation map E *and the* injection map I *the following maps:*

$$\begin{aligned} E_{N,M} \ : \ L_{T,R} &\to L_{N,M} \\ F &\mapsto (E_{N,M}F)(n,m) := F(n\delta, m\epsilon) \end{aligned} \tag{III.13}$$

$$\begin{aligned} I_{N,M} \ : \ L_{N,M} &\to L_{T,R} \\ F_{N,M} &\mapsto (I_{N,M}F_{N,M})(t,\vec{x}) := \sum_{n\in\mathbb{Z}_N, m\in\mathbb{Z}_M^D} F_{N,M}(n,m)\chi_{n\delta,m\epsilon}(t,\vec{x}) \end{aligned} \tag{III.14}$$

where $n \in \mathbb{Z}_N, m \in \mathbb{Z}_M^D$ and

$$\chi_{n\delta,m\epsilon}(t,\vec{x}) = \chi_{[n\delta,(n+1)\delta)}(t) \prod_{a=1}^{D} \chi_{m^a\epsilon,(m^a+1)\epsilon}(x^a) \tag{III.15}$$

Also, we can introduce a scalar product on $L_{N,M}$, namely

$$\langle F_{N,M}, F'_{N,M}\rangle_{N,M} := \delta\epsilon^D \sum_{n\in\mathbb{Z}_N, m\in\mathbb{Z}_M^D} F_{N,M}(n,m)F'_{N,M}(n,m) \tag{III.16}$$

As one can see, in case of the scalar field $E_{N,M} = I_{N,M}^\dagger$ where the adjoint is with respect to (III.16). However, in a more general situation, such a Hilbert space structure may not be available and in that case $E_{N,M}$ and $I_{N,M}$ are considered as independent.
One should also note that, defined in this way, these are *arbitrary* choices. In order to justify it, we note that they obey the following physically sensible properties:

Lemma III.A.1. *The evaluation and injection maps are satisfying*

[5] Indeed, while an obvious choice for studying QFT phenomena in our surroundings, nothing about this choice is imperative. We merely adopted it to simplify the bookkeeping problem in the following. Once we turn our attention towards the renormalisation of a quantum theory of Gravity, we might be interested in more irregular versions of σ. The strategy outlined in the following will still work in principle, albeit being more involved.

1. Embedding Consistency: *i.e. the embedding of an abstract lattice function carries the same information as the abstract information*

$$E_{N,M} \circ I_{N,M} = \mathrm{id}_{N,M}, \qquad I^{\dagger}_{N,M} \circ I_{N,M} = \mathrm{id}_{N,M} \tag{III.17}$$

2. Cylindrical Consistency: *i.e. the embedding of an abstract lattice function is independent on which sublattice it is defined on. For some $2 \leq p \in \mathbb{N}$, where we will pick in the following $p = 2$:*[6]

$$I_{N,M\to pN,pM} := E_{pN,pM} \circ I_{N,M}, \qquad I_{pN,pM} \circ I_{N,M\to pN,pM} = I_{N,M} \tag{III.18}$$

Proof. 1. As already mentioned for a scalar field $E_{N,M} = I^{\dagger}_{N,M}$. Then

$$(E_{N,M} \circ I_{N,M} F_{N,M})(n,m) = \sum_{n',m'} F_{N,M}(n',m')\chi_{n'\delta,m'\epsilon}(n\delta, m\epsilon) = F_{N,M}(n,m) \tag{III.19}$$

For 2. we note that for all $F_{N,M} \in L_{N,M}$ with $n' \in \mathbb{Z}_{2N},\ m' \in \mathbb{Z}^D_{2M}$

$$(I_{N,M\to 2N,2M} F_{N,M})(n',m') = F_{N,M}(\lfloor \frac{n'}{2} \rfloor, \lfloor \frac{m'}{2} \rfloor) \tag{III.20}$$

where $\lfloor . \rfloor$ denotes the component wise Gauss bracket. Now note that $M \to 2M$ implies $\epsilon = R/M \to \epsilon/2$ and hence

$$\begin{aligned}
(I_{2N,2M} \circ I_{N,M\to 2N,2M} F_{N,M})(t,\vec{x}) &= \sum_{n'\in\mathbb{Z}_{2N}, m'\in\mathbb{Z}^D_{2M}} F_{N,M}(\lfloor \frac{n'}{2} \rfloor, \lfloor \frac{m'}{2} \rfloor)\ \chi_{n'\delta/2, m'\epsilon/2}(t,\vec{x}) = \\
&= \sum_{n\in\mathbb{Z}_N, m\in\mathbb{Z}^D_M} F_{N,M}(n,m) \sum_{n'\in\mathbb{Z}_{2N}, m'\in\mathbb{Z}^D_{2M}; \lfloor n'/2 \rfloor = n, \lfloor m'/2 \rfloor = m} \chi_{n'\delta/2, m'\epsilon/2}(t,\vec{x}) = \\
&= \sum_{n\in\mathbb{Z}_N, m\in\mathbb{Z}^D_M} F_{N,M}(n,m) \sum_{r\in\{0,1\}, s\in\{0,1\}^D} \chi_{[(n+r/2)\delta, (n+r/2+\frac{1}{2})\delta)}(t) \prod_{a=1}^{D} \chi_{(m^a+s^a/2)\epsilon, (m^a+s^a/2+\frac{1}{2})\epsilon}(x^a) \\
&= \sum_{n\in\mathbb{Z}_N, m\in\mathbb{Z}^D_M} F_{N,M}(n,m)\chi_{n\delta,m\epsilon}(t,\vec{x}) = (I_{N,M}F_{N,M})(t,\vec{x})
\end{aligned} \tag{III.21}$$

□

We see that (III.16) agrees by (III.17) with the scalar product of the continuum:

$$\begin{aligned}
\langle I_{N,M}F_{N,M}, I_{N,M}F'_{N,M}\rangle &= \int dx\ (I_{N,M}F_{N,M})(I_{N,M}F'_{N,M}) = \\
&= \int dx \sum_{n,m} F_{N,M}(n,m)\chi_{n\delta,m\epsilon}(x) \sum_{n',m'} F'_{N,M}(n',m')\chi_{n'\delta,m'\epsilon}(x) \\
&= \sum_{n,n',m,m'} F_{N,M}(n,m)F'_{N,M}(n',m')\ \delta_{n,n'}\delta_{m,m'}\delta\epsilon^D = \langle F_{N,M}, F'_{N,M}\rangle_{N,M}
\end{aligned} \tag{III.22}$$

The notation for discrete fields $\Phi_{N,M}(n,m)$ smeared with discrete test functions is as usual:

$$\Phi_{N,M}[F_{N,M}] = \delta\epsilon^D \sum_{n,m} \Phi_{N,M}(n,m)F_{N,M}(n,m) \tag{III.23}$$

It suggests itself, to define a discretisation of the Weyl elements $W[F](\Phi) = \exp(i\Phi[F])$ as

$$W[I_{N,M}F_{N,M}](\Phi) =: W_{N,M}[F_{N,M}](\Phi_{N,M}) \tag{III.24}$$

Thus, upon choosing a specific injection map $I_{N,M}$ we can express everything in terms of the discrete $W_{N,M}$ on any resolution N, M. As the to-be-constructed measure $\mu_{N,M}$ is supposed to be a functional on the space of those, it transpires that the fixed point theory will depend on the choice of $I_{N,M}$.

[6]Note that the factor 2 in (III.18) bears no physical significance. It is sufficient to pick a specific value in order to construct a fixed point measure μ^*, however one could also choose any other resolution. Yet, it is not clear a priori whether the renormalisation procedure for all factors p results in the same fixed point. We will come back to this in section III.E.

III.A.2 Cylindrically Consistent Renormalisation

We will now turn towards the construction of a cylindrically consistent measure, i.e. a measure independent of the resolution used in the approximation. On $\Gamma_{N,M}$, the set of coarse history fields of resolution N, M, (i.e. for the scalar field $\Gamma_{N,M} = \mathbb{R}^{NM^D}$), a measure regular with respect to the Lebesque integral must be of the form ($O_{N,M} : \Gamma_{N,M} \mapsto \mathbb{R}$)

$$\mu(O_{N,M}) := \int_{\Gamma_{N,M}} \prod_{n,m} d\mu(\Phi(n,m))\, \rho_{N,M}(\Phi_{N,M})\, O_{N,M}(\Phi_{N,M}) \tag{III.25}$$

where ρ is some function. For example it could be chosen as the exponential of the Euclidian action

$$\rho^{(0)}_{N,M} = \exp(-S^{(0)}_{N,M}), \qquad S^{(0)}_{N,M}[\Phi_{N,M}] := S[I_{N,M}\frac{\Phi_{N,M}}{\delta\epsilon^D}] \tag{III.26}$$

However, this choice is ambiguous. There are infinitely many other choices, which like (III.26) have the property that as $N, M \to \infty$ one finds $S_{N,M}[\Phi_{N,M}] \to S[\Phi]$ where $S[\Phi]$ is the continuum Euclidian action restricted to $\mathcal{M}_{T,R}$. For any of these arbitrary choices one obtains a corresponding initial measure $\mu^{(0)}$. It is completely determined by its values on the Weyl elements, in other words the generating functional

$$\mu^{(0)}_{N,M}(W_{N,M}[F_{N,M}]) \tag{III.27}$$

This is an initial guess for a measure on coarse resolution N, M. However, it is in general not the *cylindrical projection* of the continuum measure for resolution N, M. The latter one is defined as

$$\mu_{N,M}(W_{N,M}[F_{N,M}]) := \mu(W[I_{N,M}F_{N,M}]) \tag{III.28}$$

However assuming the existence of a continuum measure, $\mu_{N,M}$ must automatically obey the following property:

Theorem III.A.1 (Projective Family). *If a measure $\mu_{N,M}$ on $\Gamma_{N,M}$ is the cylindrical projection of a continuum measure for all N, M then holds the* cylindrical consistency condition

$$\mu_{N,M}(W_{N,M}[F_{N,M}]) = \mu_{2^nN,2^mM}(W_{2^nN,2^mM}[I_{N,M\to 2^nN,2^mM}F_{N,M}]) \tag{III.29}$$

for all $F_{N,M} \in L_{N,M}$ and $N, M, n, m \in \mathbb{N}$.

Proof. For the coarse graining map $I_{N,M\to 2N,2M}$ defined in (III.18) we can establish the following consistency condition:

$$\begin{aligned} I_{2N,2M\to 4N,4M} \circ I_{N,M\to 2N,2M} &= E_{4N,4M} \circ (I_{2N,2M} \circ I_{N,M\to 2N,2M}) = \\ &= E_{4N,4M} \circ I_{N,M} = I_{N,M\to 4N,4M} \end{aligned} \tag{III.30}$$

which also implies that $\forall n, m \in \mathbb{N}$

$$I_{2^nN,2^mM} \circ I_{N,M\to 2^nN,2^mM} = I_{N,M}, \tag{III.31}$$

$$I_{2^nN2^mM\to 2^{n+n'}N,2^{m+m'}M} \circ I_{N,M\to 2^nN,2^mM} = I_{N,M\to 2^{n+n'}N,2^{m+m'}M} \tag{III.32}$$

In other words, considering a lattice function as a special continuum function is independent on what sublattice it is actually defined on.
This means for the cylindrical projections of μ:

$$\begin{aligned} \mu_{N,M}(W_{N,M}[F_{N,M}]) &= \mu(W[I_{N,M}F_{N,M}]) = \mu(W[I_{2^nN,2^mM} \circ I_{N,M\to 2^nN2^mM}F_{N,M}]) = \\ &= \mu_{2^nN,2^mM}(W_{2^nN,2^mM}[I_{N,M\to 2^nN,2^mM}F_{N,M}]) \end{aligned} \tag{III.33}$$

□

As any continuum measure implies that its cylindrical projections at coarse resolution must obey (III.28) the remaining task is to find these objects. *Renormalisation* is now merely a prescription, of how to obtain the measure μ:
Given an initial family of measures $\{\mu^{(0)}_{N,M}\}_{N,M}$ by some naive discretisation, we construct the sequence of families $(\{\mu^{(n)}_{N,M}\}_{N,M})_{n\in\mathbb{N}_0}$ inductively from $\mu^{(0)}_{N,M}$ by the so called *block spin transformation*

$$\mu^{(n+1)}_{N,M}(W_{N,M}[F_{N,M}]) := \mu^{(n)}_{2N,2M}(W_{2N,2M}[I_{N,M\to 2N,2M}F_{N,M}]) \tag{III.34}$$

Note that (III.34) indeed defines an entire new family of measures from the old one, because 1. each measure is completely defined in terms of its generating functional and 2. one performs (III.34) coherently for all M, N. Given a fixed point family $\mu^*_{N,M}$, e.g. obtained by taking the limit of $n \to \infty$ if it is convergent, we would like to relate it with a continuum measure μ^*. Note however, that in general more work could be needed, as cylindrical consistency, albeit a necessary criterion, is not sufficient to guarantee the existence of a continuum measure. An improvement of this situation will be achieved in the next section, where we develop a Hamiltonian formulation of renormalisation.

III.B Hamiltonian Renormalisation

As the idea of renormalisation was to fix the quantisation ambiguities, which arise due to a regularisation while constructing the history space measure, it is logical to use this tool also to fix the ambiguities which arise during the canonical quantisation program. Although the ambiguities presented themselves there in a totally different fashion, we already saw that there is a correspondence between the ambiguities in both schemes by the Osterwalder-Schrader reconstruction and its inverse the OS construction.

In order to fix the quantisation ambiguities in the Hamiltonian formulation of a quantum theory, one could hence go to the corresponding covariant formalism, construct a fixed point measure μ^* and perform OS reconstruction to obtain back the Hamiltonian framework. This is what is usually done in the literature. The idea of this thesis is now to circumvent the construction of the history space time measure by transferring the formalism of renormalisation directly into the Hamiltonian framework. Instead of performing the search for a fixed point of (III.34) for the OS measure μ we try to find an equivalent renormalisation condition for the OS data $(\mathcal{H}, \hat{H}, \Omega)$. This equivalent condition will be developed in the first subsection, by making the diagram in figure III.1 close.

Albeit it is possible to develop such a scheme (following the derivation from [128]), it will transpire that the construction of the measure is needed as an intermediate step! Hence, the framework fails at its original aim of simplifying the search for a discretisation error free quantum theory. Yet it motivates a renormalisation scheme for a purely Hamiltonian renormalisation, which will also yield as fixed points cylindrically consistent theories[7]. This alternative scheme was developed in [128] and we quote their results in the second subsection.

III.B.1 Path-Integral (PI) induced Hamiltonian Renormalisation

We assume that we are given a family of naively discretised canonical quantum theories described by the OS data $(\mathcal{H}_M^{(0)}, \hat{H}_M^{(0)}, \Omega_M^{(0)})$ labelled by M. Since the Hamiltonian is the generator of a contraction semi-group with a continuous parameter, time takes necessarily a special role. By the OS construction we obtain a corresponding measure family $\mu_M^{(0)}$, which has still spatially discrete support, while continuous in time. Hence, we can define from this the cylindrical projections $\mu_{N,M}^{(0)}$ for finite time resolutions labelled by N in the spirit of (III.28) by introducing an injection map I_N purely for temporal functions. This however implies that the history space measure is already cylindrically consistent in time. In other words: starting with the OS data we obtain a measure where the renormalisation in time direction has already been taken care of!
For the remainder of this section, we will thus assume that all measures involved are renormalised in time.

We begin by introducing purely spatial injections maps $I_M: L_M \to L_R$ for each M. They are satisfying the conditions from Lemma III.A.1.

Lemma III.B.1. *The spatial block spin transformation induced by the map $I_{M\to 2M}$ defined from I_M by (III.18) maps OS measures $\mu_M^{(n)}$ to OS measures via*

$$\mu_M^{(n+1)}(W_M[F_M]) := \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}F_M]) \tag{III.35}$$

for all $F_M \in [0,T) \times L_M$[8]. In other words it does not leave the space of time translation invariant, reflection invariant and reflection positive measures.

Proof. As $I_{M\to 2M}$ acts at each time step only on the spatial arguments of F_M, it commutes with time reflection θ and time translation T_s defined in (II.152).
Thus follows time translation invariance:

$$\begin{aligned}\mu_M^{(n+1)}(\mathcal{U}(s)W_M[F_M]) &= \mu_M^{(n+1)}(W_M[T_sF_M]) = \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}T_sF_M]) = \mu_{2M}^{(n)}(W_{2M}[T_sI_{M\to 2M}F_M]) \\ &= \mu_{2M}^{(n)}(\mathcal{U}(s)W_{2M}[I_{M\to 2M}F_M]) = \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}F_M]) = \mu_M^{(n+1)}(W_M[F_M])\end{aligned} \tag{III.36}$$

[7]The price to pay for this new Hamiltonian renormalisation scheme is, that the set of fixed points obtained as the limit $n \to \infty$ of some naive discretised theory might be very different from the fixed points of the measure induced renormalisation. In the later discussed example of the free field one can see that the fixed points agree, however the trajectories in "theory space" leading to them will differ.

[8]Note that we could also consider F_M depending on multiple times, $F_M \in [0,T)^n \times L_M$. By decomposing into several Weyl elements at each coinciding point of time however it is sufficient to show the invariance of the new measure for only one time dependence.

Time reflection invariance:

$$\mu_M^{(n+1)}(R\,W_M[F_M]) = \mu_M^{(n+1)}(W_M[\theta F_M]) = \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}\theta F_M]) = \mu_{2M}^{(n)}(W_{2M}[\theta I_{M\to 2M} F_M]) = \\ = \mu_{2M}^{(n)}(R\,W_{2M}[I_{M\to 2M}F_M]) = \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}F_M]) = \mu_M^{(n+1)}(W_M[F_M]) \tag{III.37}$$

Reflection Positivity:

$$\mu_M^{(n+1)}(W_M[F_M]^*(R\,W_M[F_M])) = \sum_\alpha z_\alpha \mu_M^{(n+1)}(W_M[F_{\alpha,M}(F_M^*, \theta F_M)]) = \\ = \sum_\alpha z_\alpha \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}F_{\alpha,M}(F_M^*, \theta F_M)]) = \sum_\alpha z_\alpha \mu_{2M}^{(n)}(W_{2M}[F_{\alpha,M}((I_{M\to 2M}F_M)^*, \theta I_{M\to 2M}F_M)]) \\ = \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}F_M])^*(R\,W_M[I_{M\to 2M}F_M])) \geq 0 \tag{III.38}$$

where we used the Weyl relations (II.98) and that for a free scalar field

$$I_{M\to 2M}F_M^* = (I_{M\to 2M}F_M)^*, \qquad I_{M\to 2M}F_{\alpha,M}(F_M, F_M') = F_{\alpha,M}(I_{M\to 2M}F_M, I_{M\to 2M}F_M') \tag{III.39}$$

which is easily verified, using $F^* = -F$ and $F_\alpha(f, f') = f + f'$ and linearity of $I_{M\to 2M}$. . ☐

Consequently, we know that we can indeed use the OS reconstruction to obtain new OS data, which we call accordingly $(\mathcal{H}_M^{(n+1)}, \hat{H}_M^{(n+1)}, \Omega_M^{(n+1)})$.
In the OS reconstruction of a measure $\mu_M^{(n)}$ the Hilbert space $\mathcal{H}_M^{(n)}$ is the closure of the equivalence classes $[.]_{\mu_M^{(n)}}$ of Ψ with respect to the Null space $\mathcal{N}$ induced by $\mu_M^{(n)}$. The Ψ are here the finite linear combination of the Weyl elements $W_M[F_M]$ with $\mathrm{T}-\mathrm{supp}(F) \subset \mathbb{R}_+$, i.e. of positive time support. Let us hence define a map between two Hilbert spaces, neighbouring in the renormalisation sequence:

$$\begin{array}{rrcl} J_{M\to 2M}^{(n)} : & \mathcal{H}_M^{(n+1)} & \to & \mathcal{H}_{2M}^{(n)} \\ & [W_M[F_M]]_{\mu_M^{(n+1)}} & \mapsto & [W_{2M}[I_{M\to 2M}F_M]]_{\mu_{2M}^{(n)}} \end{array} \tag{III.40}$$

Being defined on a dense domain in $\mathcal{H}_M^{(n+1)}$, its action generalises straightforwardly to the closure.

Lemma III.B.2. *The map $J_{M\to 2M}^{(n)}$ as given by (III.40) defines for each n an isometric embedding, i.e.*

$$(J_{M\to 2M}^{(n)})^\dagger J_{M\to 2M}^{(n)} = \mathrm{id}_{\mathcal{H}_M^{(n+1)}} \tag{III.41}$$

Hence

$$P_{2M}^{(n)} := J_{M\to 2M}^{(n)}(J_{M\to 2M}^{(n)})^\dagger \tag{III.42}$$

are projectors for each n onto the subspace $J_{M\to 2M}^{(n)}\mathcal{H}_M^{(n+1)} \subset \mathcal{H}_{2M}^{(n)}$, i.e.

$$(P_{2M}^{(n)})^2 = P_{2M}^{(n)}, \qquad P_{2M}^{(n)}J_{M\to 2M}^{(n)} = J_{M\to 2M}^{(n)}, \qquad (J_{M\to 2M}^{(n)})^\dagger P_{2M}^{(n)} = (J_{M\to 2M}^{(n)})^\dagger \tag{III.43}$$

Proof. We compute the scalar product as given in the OS reconstruction between two Weyl elements in $\mathcal{H}_M^{(n+1)}$ to show the isometry of $J_{M\to 2M}^{(n)}$: (we make use of the Weyl relations for the second line)

$$\langle [W_M[F_M]]_{\mu_M^{(n+1)}}, [W_M[F_M']]_{\mu_M^{(n+1)}} \rangle_{\mathcal{H}_M^{(n+1)}} = \mu_M^{(n+1)}((W_M[F_M])^* W_M[\theta F_M']) = \\ = \mu_{2M}^{(n)}((W_{2M}[I_{M\to 2M}F_M])^* W_{2M}[\theta I_{M\to 2M}F_M']) = \langle [W_{2M}[I_{M\to 2M}F_M]]_{\mu_{2M}^{(n)}}, [W_{2M}[I_{M\to 2M}F_M']]_{\mu_{2M}^{(n)}} \rangle_{\mathcal{H}_{2M}^{(n)}} \\ = \langle J_M^{(n)}[W_M[F_M]]_{\mu_M^{(n+1)}}, J_M^{(n)}[W_M[F_M']]_{\mu_M^{(n+1)}} \rangle_{\mathcal{H}_{2M}^{(n)}} \tag{III.44}$$

The properties of the projection $P_{2M}^{(n)}$ follow now straightforwardly:

$$(P_{2M}^{(n)})^2 = J_{M\to 2M}^{(n)}((J_{M\to 2M}^{(n)})^\dagger J_{M\to 2M}^{(n)})(J_{M\to 2M}^{(n)})^\dagger = P_{2M}^{(n)} \tag{III.45}$$

The other two follow similarly. ☐

Lemma III.B.3. *The determining equation for the Hamiltonian after a renormalisation step reads: ($\beta > 0$)*

$$e^{-\beta \hat{H}_M^{(n+1)}} = (J^{(n)}_{M\to 2M})^\dagger e^{-\beta \hat{H}^{(n)}_{2M}} J^{(n)}_{M\to 2M} \tag{III.46}$$

Proof. We show the property for arbitrary matrix elements in a dense domain:

$$\begin{aligned}
&\langle [W_M[F_M]]_{\mu_M^{(n+1)}}, e^{-\beta \hat{H}_M^{(n+1)}} [W_M[F'_M]]_{\mu_M^{(n+1)}} \rangle_{\mathcal{H}_M^{(n+1)}} = \mu_M^{(n+1)}((W_M[F_M])^* W_M[\theta T_\beta F'_M]) = \\
&= \mu_{2M}^{(n)}((W_{2M}[I_{M\to 2M}F_M])^* W_{2M}[I_{M\to 2M}\theta T_\beta F'_M]) = \mu_{2M}^{(n)}((W_{2M}[I_{M\to 2M}F_M])^* W_{2M}[\theta T_\beta I_{M\to 2M} F_M]) \\
&= \langle [W_{2M}[I_{M\to 2M}F_M]]_{\mu_{2M}^{(n)}}, e^{-\beta \hat{H}_{2M}^{(n)}} [W_{2M}[I_{M\to 2M}F'_M]]_{\mu_{2M}^{(n)}} \rangle_{\mathcal{H}_{2M}^{(n)}} = \\
&= \langle J^{(n)}_{M\to 2M}[W_M[F_M]]_{\mu_{2M}^{(n+1)}}, e^{-\beta \hat{H}_{2M}^{(n)}} J^{(n)}_{M\to 2M}[W_M[F'_M]]_{\mu_M^{(n+1)}} \rangle_{\mathcal{H}_{2M}^{(n)}}
\end{aligned} \tag{III.47}$$

□

Equation (III.46) incorporates a lot of information. For once setting $\beta = 0$ recovers the isometry condition for $J^{(n)}_{M\to 2M}$. Moreover taking the l-th derivative and afterwards evaluating at $\beta = 0$ yields

$$(\hat{H}_M^{(n+1)})^l = (J^{(n)}_{M\to 2M})^\dagger (\hat{H}^{(n)}_{2M})^l J^{(n)}_{M\to 2M} \tag{III.48}$$

For $l = 1$ it transpires that the whole sequence of Hamiltonians and hence also the limit fixed point will be symmetric if the initial discretisations are. Moreover it seems that this equation should be sufficient to determine $\hat{H}_M^{(n+1)}$, however there are additional conditions arising for further $l \geq 2$. For example there are two ways we can express $(\hat{H}_M^{(n+1)})^2$ by combining $l = 1$ and $l = 2$:

$$(J^{(n)}_{M\to 2M})^\dagger (\hat{H}^{(n)}_{2M})^2 J^{(n)}_{M\to 2M} = (J^{(n)}_{M\to 2M})^\dagger \hat{H}^{(n)}_{2M} P^{(n)}_{2M} \hat{H}^{(n)}_{2M} J^{(n)}_{M\to 2M} \tag{III.49}$$

Multiplying this with $(J^{(n)}_{M\to 2M})^\dagger$ from the right and with $J^{(n)}_{M\to 2M}$ from the left yields

$$P^{(n)}_{2M} (\hat{H}^{(n)}_{2M})^2 P^{(n)}_{2M} = P^{(n)}_{2M} \hat{H}^{(n)}_{2M} P^{(n)}_{2M} \hat{H}^{(n)}_{2M} P^{(n)}_{2M} \tag{III.50}$$

which is equivalent to

$$\begin{aligned}
0 &= P^{(n)}_{2M} \hat{H}^{(n)}_{2M} (\mathrm{id}_{\mathcal{H}^{(n)}_{2M}} - P^{(n)}_{2M}) \hat{H}^{(n)}_{2M} P^{(n)}_{2M} = P^{(n)}_{2M} \hat{H}^{(n)}_{2M} [P^{(n)}_{2M}]^\perp \hat{H}^{(n)}_{2M} P^{(n)}_{2M} = \\
&= (P^{(n)}_{2M} \hat{H}^{(n)}_{2M} [P^{(n)}_{2M}]^\perp)(P^{(n)}_{2M} \hat{H}^{(n)}_{2M} [P^{(n)}_{2M}]^\perp)^\dagger =: A^\dagger A
\end{aligned} \tag{III.51}$$

where we used that $[P^{(n)}_{2M}]^\perp = ([P^{(n)}_{2M}]^\perp)^2$ is also a projection towards the orthogonal complement.
It follows that for all $\Psi \in \mathcal{H}^{(n)}_{2M}$ we have $\langle \Psi, A^\dagger A \Psi \rangle = ||A\Psi||^2 = 0$ thus $A \equiv 0$. Consequently using first $A^\dagger = 0$ and then $A = 0$ we get

$$\hat{H}^{(n)}_{2M} P^{(n)}_{2M} = P^{(n)}_{2M} \hat{H}^{(n)}_{2M} P^{(n)}_{2M} = (P^{(n)}_{2M} \hat{H}^{(n)}_{2M} P^{(n)}_{2M})^\dagger = P^{(n)}_{2M} \hat{H}^{(n)}_{2M} \tag{III.52}$$

In summary we see that $[\hat{H}^{(n)}_{2M}, P^{(n)}_{2M}] = 0$ hence $\hat{H}^{(n)}_{2M}$ preserves the subspace $P^{(n)}_{2M}\mathcal{H}^{(n)}_{2M}$.

A consequence of this relation is that one must (at least for the free field) think of the elements in $\mathcal{H}^{(n)}_M$ for example either as single field species at an increasing number of time (as $n \to \infty$) or multiple interacting field species, but not as vectors in the span generated by the sharp time zero fields acting on $\Omega^{(n)}_M$.
We assume that would be not the case, then, at some n, a representative of the equivalence class is given as

$$[W_M[F_M]]_{\mu_M^{(n)}} = \sum_{k=1}^N \lambda_k w_M[f_{M,k}] \Omega_M^{(n)} \tag{III.53}$$

with the spatial Weyl elements w_M at sharp time zero, some smearing functions $f_{M,k}$ and $\lambda_k \in \mathbb{C}$. Then follows

$$J^{(n)}_{M\to 2M}[[W_M[F_M]]_{\mu_M^{(n)}} = \sum_{k=1}^N \lambda_k w_M[I_{M\to 2M}[f_{M,k}]] \Omega_M^n \tag{III.54}$$

i.e. for each $m \in \mathbb{Z}_M^D$ the excitation on all $m' \in \mathbb{Z}_{2M}^D$ with $\lfloor \frac{m'}{2} \rfloor = m$ will be the same. (III.52) implies now, that this property will not change under time evolution, in other words if the field is constant on a block of coarse resolution with respect to a fine lattice it will never develop excitations that could only be resolved with the mentioned finer resolution. This property is certainly violated for the cylindrical projections of a continuum theory.

We study this complications that arise due to the presence of the equivalence class $[.]_{\mu_M^{(n)}}$ later in the example of the free field: Albeit starting with $\mathcal{H}_M^{(0)}$ being the span of sharp time zero fields, already after one renormalisation step this will be no longer the case. Instead, we could label $[[W_M[F_M]]_{\mu_M^{(n)}}$ for the free field as spatial Weyl elements at an increasing number of sharp times as $n \to \infty$. Due to this, however, the $\mathcal{H}_M^{(n)}$ do not qualify immediately as cylindrical projections by I_M of a continuum Hilbert space spanned by the continuum $w[f]\Omega$. The dependence of the equivalence class is crucial for determining the structure of the new Hilbert space $\mathcal{H}_M^{(n+1)}$ during the renormalisation sequence. However this means we do not acquire the wanted simplification regarding the renormalisation procedure, as we have to compute the history space measure $\mu_M^{(n+1)}$ at each intermediate step in order to determine the new Hilbert space $\mathcal{H}_M^{(n+1)}$.
This drawback motivates to define a new renormalisation prescription which stays completely in the Hamiltonian framework and is simpler to execute, which we will present in the next subsection. But before we continue with this, let us lastly summarise the *path-integral induced Hamiltonian renormalisation*:

1. Pick an initial discretisation family $(\mathcal{H}_M^{(0)}, \hat{H}_M^{(0)}, \Omega_M^{(0)})$, labelled by M. Determine the history space measure $\mu_M^{(0)}$ via OS construction.
2. Determine the family $\mu_M^{(n+1)}$ via
$$\mu_M^{(n+1)}(W_M[F_M]) := \mu_{2M}^{(n)}(W_{2M}[I_{M\to 2M}F_M]) \ . \tag{III.55}$$
Use this to define the equivalence class $[.]_{\mu_M^{(n+1)}}$ of the OS reconstruction and give rise to a map $J_{M\to 2M}^{(n)}$ such that it embeds $\mathcal{H}_M^{(n+1)}$ into $\mathcal{H}_{2M}^{(n)}$.
3. Set $\Omega_M^{(n+1)} = [1]_{\mu_M^{(n+1)}} = (J_{M\to 2M}^{(n)})^\dagger \Omega_{2M}^{(n)}$. Let $\mathcal{H}_M^{(n)}$ be the span of the $[W_M[F_M]]_{\mu_M^{(n+1)}}$. Determine the Hilbert space measure $d\nu_M^{(n)}$ by demanding that $J_{M\to 2M}^{(n)}$ is an isometry. Set
$$\hat{H}_M^{(n+1)} = (J_{M\to 2M}^{(n)})^\dagger \hat{H}_{2M}^{(n)} J_{M\to 2M}^{(n)} \ . \tag{III.56}$$
4. Start over at step 2 until you run into a fixed point $(\mathcal{H}_M^*, \hat{H}_M^*, \Omega_M^*)$ and μ_M^* for $n \to \infty$.

III.B.2 Direct Hamiltonian Renormalisation

Assuming a canonical quantum field theory in the continuum $(\mathcal{H}, \hat{H}, \Omega)$ on a compactified manifold $\sigma_R = [0,R)^D$, we might look at its projections onto a discretised spatial manifold, e.g. $\sigma_M = \mathbb{Z}_M^D$. We can follow the construction of observables outlined above: Like in (III.12) we call the spatially discretised fields

$$\phi_M(m) := \phi[\chi_{m\epsilon}], \qquad w_M[f_M](\phi_M) := w[I_M f_M](\phi) = \exp(i\phi[I_M f_M]) \tag{III.57}$$

where $\epsilon = \epsilon_M$ and $\in \mathbb{Z}_M^D$, $f_M \in L_M$. We had also already introduced the spatial injection maps I_M. It follows that the cylindrical projections ν_M of the continuum Hilbert space measure ν (which describes the scalar product on $\mathcal{H}$) must also represent a projective family following theorem III.A.1, i.e. $\forall n \in \mathbb{N}$

$$\nu_M(w_M[f_M]) = \nu_{2^n M}(w_{2^n M}[I_{M\to 2^n M} f_M]) \tag{III.58}$$

Moreover, let us introduce the map $j_M : \mathcal{H}_M \to \mathcal{H}$ with $j_M w_M[f_M] \mapsto w[I_M f_M]$. Since the continuum theory exists, we can compute the matrix elements of the continuum Hamiltonian on observables of coarse resolution M and use this to define an operator $\hat{H}_M$ on the lattice: $\forall f, f' \in L_M$

$$\langle w[I_M f'_M]\Omega, \hat{H} w[I_M f_M]\Omega\rangle_{\mathcal{H}} = \langle w_M[f'_M]\Omega_M, j_M^\dagger \hat{H} j_M w_M[f_M]\Omega_M\rangle_{\mathcal{H}_M} =: \langle w_M[f'_M]\Omega_M, \hat{H}_M w_M[f_M]\Omega_M\rangle_{\mathcal{H}_M} \tag{III.59}$$

with $\Omega_M := j_M \Omega$. These realisations lead us to the following definition of a direct Hamiltonian renormalisation: We follow in our notation closely the notation introduced in the previous section, so the reader may see how slightly yet crucially they differ:

Starting from initial OS data $(\mathcal{H}_M^{(0)}, \hat{H}_M^{(0)}, \Omega_M^{(0)})$ where $\mathcal{H}_M^{(0)}$ is spanned by the spatial Weyl elements $w_M[f_M]$, we define the maps

$$\begin{aligned} j_{M\to 2M}^{(n)} \ :\ \mathcal{H}_M^{(n+1)} \quad &\to\ \mathcal{H}_{2M}^{(n)} \\ w_M[f_M]\Omega_M^{(n+1)}\ &\mapsto\ w_{2M}[I_{M\to 2M}f_M]\Omega_{2M}^{(n)} \end{aligned} \tag{III.60}$$

Hence we can straightforward identify for the vacuum vector (by setting $f_M = 0$) that

$$j_{M\to 2M}^{(n)}\Omega_M^{(n+1)} = \Omega_{2M}^{(n)} \tag{III.61}$$

Without any recourse to a history space measure, the map $j_{M\to 2M}^{(n)}$ is right now largely arbitrary as we have not fixed anything. We now demand two conditions for $j_{M\to 2M}^{(n)}$, which in order to be fulfilled will determine for each step n the exact form of the OS data of step $n+1$.

Definition III.B.1. *We call the map $j_{M\to 2M}^{(n)}$ defined by (III.60) a* renormalisation isometry *iff*

1. *it is isometric, i.e.*

$$(j_{M\to 2M}^{(n)})^\dagger j_{M\to 2M}^{(n)} = \mathrm{id}_{\mathcal{H}_M^{(n+1)}} \tag{III.62}$$

2. *it determines the flow of the Hamiltonian (and keeps it symmetric), i.e.*

$$\hat{H}_M^{(n+1)} := (j_{M\to 2M}^{(n)})^\dagger \hat{H}_M^{(n)} j_{M\to 2M}^{(n)} \tag{III.63}$$

It is easy to see that (III.62) induces the mentioned cylindrical consistency condition (III.58) for the Hilbert space measure. Recall for this that $\nu_M(\ .\ ) = \langle \Omega_M,\ .\ \Omega_M\rangle_{\mathcal{H}_M}$. (III.63) is the sufficient part of the stronger condition (III.46), however without imposing the remaining conditions. This helps us in circumventing that the field content changes. Note also that this condition *defines* the operator on $\mathcal{H}_M^{(n+1)}$ which has exactly the same matrix elements as the Hamiltonian $\hat{H}_{2M}^{(n)}$ when projected, which is a necessary condition in order to be the coarse version of a continuum Hamiltonian as discussed in (III.59).

We want to also to remark that the flow between Hamiltonians and vacua is consistent since

$$\hat{H}_M^{(n+1)}\Omega_M^{(n+1)} = (j_{M\to 2M}^{(n)})^\dagger \hat{H}_{2M}^{(n)} j_{M\to 2M}^{(n)}\Omega_M^{(n+1)} = (j_{M\to 2M}^{(n)})^\dagger \hat{H}_{2M}^{(n)}\Omega_{2M}^{(n)} = 0 \tag{III.64}$$

Let us finish this section with a quick summary of the *direct Hamiltonian renormalisation*:

1. Pick an initial discretisation family $(\mathcal{H}_M^{(0)}, \hat{H}_M^{(0)}, \Omega_M^{(0)})$ labelled by M and $\mathcal{H}_M^{(0)}$ spanned by $w_M[f_M]\Omega_M$.
2. Set $\Omega_M^{(n+1)} = (j_{M\to 2M}^{(n)})^\dagger \Omega_{2M}^{(n)}$. Set $\mathcal{H}_M^{(n+1)} = span\{w_{2M}[I_{M\to 2M}f_M]\Omega_M;\ f_M \in L_M\}$. Set

$$\nu_M^{(n+1)}(w_M[f_M]) := \nu_{2M}^{(n)}(w_{2M}[I_{M\to 2M}f_M]) \tag{III.65}$$

   and for the Hamiltonian

$$\hat{H}_M^{(n+1)} = (j_{M\to 2M}^{(n)})^\dagger \hat{H}_{2M}^{(n)} j_{M\to 2M}^{(n)} \tag{III.66}$$

3. Start over at step 2 until you run into a fixed point $(\mathcal{H}_M^*, \hat{H}_M^*, \Omega_M^*)$ for $n\to\infty$.

III.B.3 Relating to the Continuum via inductive Limits

Above scheme was derived assuming the existence of a continuum theory and motivated by staying as close as possible to the path-integral induced scheme. To re-establish contact with the continuum, after having found the discrete cylindrically consistent theories, we would hope to understand the family of Hilbert spaces as an *inductive limit*. There are excellent accounts in the literature [140–146] so we will only briefly collect the basic notions of inductive limits and apply them to our case by quoting from [128].

Definition III.B.2. *Let $(\mathcal{I},<)$ be a partially ordered index set. We call a system of Hilbert spaces $\{\mathcal{H}_i\}_{i\in\mathcal{I}}$ an* inductive system of Hilbert spaces *iff for each $i<j$ there exist isometric injections*

$$J_{i\to j}\;:\;\mathcal{H}_i\to\mathcal{H}_j \tag{III.67}$$

with $J_{i\to i}=\mathrm{id}_{\mathcal{H}_i}$ and consistency $J_{i\to k}=J_{j\to k}\circ J_{i\to j}$ for all $i<j<k$.
A family of operators $\{A_i\}_{i\in\mathcal{I}}$ with dense and invariant domains D_i is called inductive system of operators *iff for $i<j$*

$$J_{i\to j}D_i\subset D_j,\;\;A_jJ_{i\to j}=J_{i\to j}A_i \tag{III.68}$$

Lemma III.B.4. *1. For every inductive system of Hilbert spaces there exists a unique (up to unitary equivalence) Hilbert space $\mathcal{H}$ and isometric injections $J_i:\mathcal{H}_i\to\mathcal{H}$ for each $i\in\mathcal{I}$ such that for all $i<j$*

$$J_jJ_{i\to j}=J_i \tag{III.69}$$

2. For every inductive system of operators there exists an operator A on a dense $D\subset\mathcal{H}$, with $J_iD_i\subset D$, such that $\forall i\in\mathcal{I}$:

$$J_i\;A_i=A\;J_i \tag{III.70}$$

If, moreover, every A_i is essentially self-adjoint with core D_i then so is A on D.

Proof. 1. We call vectors $\psi_i\in\mathcal{H}_i,\;\psi_j\in\mathcal{H}_j$ equivalent iff there exists k such that for any $i,j<k$ we have $J_{i\to k}\psi_i=J_{j\to k}\psi_j$. Indeed, when it is true for one k it holds for all $k'\in\mathcal{I}$: Take $l>k,k'$ then by equivalence for k we have

$$0=J_{k\to l}(J_{i\to k}\psi_i-J_{j\to k}\psi_j)=J_{i\to l}\psi-J_{j\to l}\psi_j=J_{k'\to l}(J_{i\to k'}\psi_i-J_{j\to k'}\psi_j) \tag{III.71}$$

However, since isometries are automatically injective it follows: $J_{i\to k'}\psi_i=J_{j\to k'}\psi_j$. We consider the equivalence classes $[\psi_i]$ and equip them with the inner product

$$\langle[\psi_i],[\psi_j]\rangle_{\mathcal{H}}:=\langle J_{i\to k}\psi_i,J_{k\to j}\psi_j\rangle_{\mathcal{H}_k} \tag{III.72}$$

where k is any $i,j<k$. This is independent of the representative because for any $i,j<k'$ we find $k,k'<l$ and have by isometry and consistency:

$$\begin{aligned}\langle J_{i\to k}\psi_i,J_{j\to k}\psi_j\rangle_{\mathcal{H}_k}&=\langle J_{k\to l}J_{i\to k}\psi_i,J_{k\to l}J_{j\to k}\psi_j\rangle_{\mathcal{H}_l}=\langle J_{i\to l}\psi_i,J_{j\to l}\psi_j\rangle_{\mathcal{H}_l}=\\&=\langle J_{k'\to l}J_{i\to k'}\psi_i,J_{k'\to l}J_{j\to k'}\psi_j\rangle_{\mathcal{H}_l}=\langle J_{i\to k'}\psi_i,J_{j\to k'}\psi_j\rangle_{\mathcal{H}_{k'}}\end{aligned} \tag{III.73}$$

The inductive limit Hilbert space $\mathcal{H}$ is now the completion of the formal finite linear combinations of equivalence classes.
The required maps can be defined as

$$J_i\psi_i:=[\psi_i] \tag{III.74}$$

Then, we have indeed for any $i<j$:

$$J_jJ_{i\to j}\psi_i=[J_{i\to j}\psi_i]=[\psi_j]=[\psi_i]=J_i\psi_i \tag{III.75}$$

where we used that ψ_i and $\psi_j=J_{i\to j}\psi_i$ are equivalent (choose $k=j>i$). The J_i are injections since $J_i\psi_i=[\psi_i]=0$ means that $J_{i\to j}\psi_i=0$ for some $i<j$ hence $\psi_i=0$. they are also isometric since (pick $k=i$)

$$\langle J_i\psi_i,J_i\psi_i\rangle_{\mathcal{H}}=\langle[\psi_i],[\psi_i']\rangle_{\mathcal{H}}=\langle\psi_i,\psi_i'\rangle_{\mathcal{H}_i} \tag{III.76}$$

Thus, it remains to show uniqueness up to unitary equivalence. For this, assume that two inductive limits $(\mathcal{H},\{J_i\}_{i\in\mathcal{I}})$ and $(\mathcal{H}'\{J_i'\}_{i\in\mathcal{I}})$ have been found. We define

$$\begin{aligned}U\;:\;\mathcal{H}\;\to\;\mathcal{H}'\\J_i'\psi_i\mapsto J_i\psi_i\end{aligned} \tag{III.77}$$

and extend by linearity to the dense domain of the finite linear combinations of the $J_i\psi_i$. It has the inverse on its image: $U^{-1}(J'_i\psi_i) = J_i\psi_i$ and is isometric (pick any $i, j < k$)

$$\langle UJ_i\psi_i, UJ_j\psi_j\rangle_{\mathcal{H}'} = \langle J'_i\psi_i, J'_j\psi_j\rangle_{\mathcal{H}'} = \langle J'_kJ_{i\to k}\psi_i, J'_kJ_{j\to k}\psi_j\rangle_{\mathcal{H}'} = \langle J_{i\to k}\psi_i, J_{j\to k}\psi_k\rangle_{\mathcal{H}_k} = \langle J_i\psi_i, J_j\psi_j\rangle_{\mathcal{H}} \tag{III.78}$$

and can therefore be extended to a unitary operator to all of $\mathcal{H}$ by continuity.
2. We define D to be the finite linear combinations of the vectors $J_i\psi_i,\ \psi_i \in D_i$. As the D_i are dense in $\mathcal{H}_i$ it follows that D is dense in $\mathcal{H}$. Then we *define* and extend by linearity

$$A\,(J_i\psi) := J_i\ A_i\ \psi_i \tag{III.79}$$

This definition is consistent for suppose that $J_i\psi_i = J_j\psi_j$ then for $i, j < k$ it is $J_{i\to k}\psi_i = J_{j\to k}\psi_j$ and

$$A(J_i\psi_i - J_j\psi_j) = A(J_kJ_{i\to k}\psi_i - J_kJ_{j\to k}\psi_j) = J_kA_k(J_{i\to k}\psi_i - J_{j\to k}\psi_j) = 0 \tag{III.80}$$

Finally, by the basic criterion of essential self-adjointness, we know that $(A_j \pm i\ \mathrm{id}_{\mathcal{H}_j})D_j$ is dense in $\mathcal{H}_j$. It follows that for any j

$$(A \pm i\ \mathrm{id}_{\mathcal{H}})J_jD_j = J_j(A_j \pm i\ \mathrm{id}_{\mathcal{H}_j})D_j \tag{III.81}$$

is dense in J_jD_j, hence $(A \pm i\ \mathrm{id}_{\mathcal{H}_j})D$ is dense in $\mathcal{H}$ and A is essentially self-adjoint. □

These concepts of inductive limits are now applicable in the context of renormalisation of theories, as upon having found a fixed point $(\mathcal{H}^*_M, \hat{H}^*_M, \Omega^*_M)$ by the direct Hamiltonian renormalisation the maps $j_{M\to 2M}$ give rise to the concatenations

$$j_{M\to 2^nM} := j_{2^{n-1}M\to 2^nM} \circ \dots \circ j_{M\to 2M} \tag{III.82}$$

which are satisfying the conditions of (III.67). There are numerous partially ordered and directed label sets in this case, namely $\mathcal{I}_k = \{M := (2k+1)2^n,\ n \in \mathbb{N}_0\}$ for each $k \in \mathbb{N}_0$. Hence the existence of the continuum Hilbert space $\mathcal{H}^k$ is guaranteed by the previous Lemma, as well as the existence of embedding maps $j_M :\ \mathcal{H}_M \to \mathcal{H}^k$. If there is no dependence on k, i.e. $\mathcal{H} = \mathcal{H}^k\ \forall k$, we call the theory *partially universal*.[9]
However, it is important to point out that while we have determined a family of perfect discretised Hamiltonian operators obeying

$$j^\dagger_{M\to M'}\hat{H}_{M'}j_{M\to M'} = \hat{H}_M \tag{III.83}$$

for all $M < M'$, this condition is *not* equivalent with (III.68), i.e. the condition which would have guaranteed the existence of a continuum Hamiltonian operator. Sadly, the latter condition is stronger than the one we obtain from the Hamiltonian renormalisation, hence we are not obtaining a continuum Hamiltonian operator via this prescription. Instead, we can construct a consistently defined symmetric quadratic form. Under certain assumptions, we can hope to find its Friedrichs extension as a self-adjoint positive operator [186].
Hence, the situation in the direct Hamiltonian renormalisation is equally good as in the standard renormalisation of a spacetime measure, where cylindrical consistency is a necessary criterion as well.

[9] We will later see an example for partially universality in case of the free field.

III.C Example: Klein Gordon field I - Derivation

In order to make the above formalism concrete we will know study a concrete example, namely the massive free scalar field, also known as Klein Gordon field. Its continuum quantum theory has been excessively studied in section II.D of the last chapter. Now we will artificially discretise it and study whether the fixed point theory obtained via both renormalisation schemes yields an inductive limit Hamiltonian which agrees with the known continuum dynamics. By this we put both renormalisation prescriptions to a necessary test, which both will pass: We will explicitly determine the corresponding fixed point structure and show that the resulting Hamiltonian theories indeed correspond to the continuum theories constructed earlier.

Hence, we introduce as described above a spatial IR cut-offs R and work on finite lattices with M points in each spatial direction. We introduce maybe a natural but still ad hoc discretised version of the Hamiltonian and apply both the renormalisation procedures derived in the previous sections. For this, we can copy the calculations from [129] and will do so in the following.

The common starting point for both renormalisation trajectories is a family of either Gaussian, reflection positive measures $\mu_M^{(0)}$ or equivalently OS data $(\mathcal{H}_M^{(0)}, \hat{H}_M^{(0)}, \Omega_M^{(0)})$ originating from some spatial (lattice) discretisation of the classical continuum theory. In what follows, we construct such a discretisation explicitly using a choice of the coarse graining map.
The fields at finite IR cut-off are supposed to obey periodic boundary conditions and the corresponding one particle Hilbert space is $L_R := L_2([0,R)^D, d^Dx)$. In the presence of an additional UV cut-off we define the one particle Hilbert space as $L_{RM} := \ell_2(\mathbb{Z}_M^D)$ with $\mathbb{Z}_M := \{0,1,..,M-1\}$. These are the square summable finite sequences f_{RM} with norm squared

$$||f_M||^2_{L_M} := \epsilon_M^D \sum_{m\in\mathbb{Z}_M^D} |f_M(m)|^2, \;\; \epsilon_M := \frac{R}{M} \tag{III.84}$$

which is the spatial version of (III.16). In this chapter we explicitly state the dependence of the lattice spacing on M, i.e. $\epsilon = \epsilon_M$. Not also that the prefactor ϵ_M^D is consistent with the interpretation that $f_M(m) = f(m\epsilon_M)$ for some $f \in L_R$ so that $||f_M||_{L_M} = ||f||_{L_R}$.
Using the spatial injections I_M and evaluations E_M we already established for (III.35), we consider the discretised classical fields

$$\phi_M(m) := (I_M^\dagger \phi)(m) = \int_{[0,R)^D} d^Dx \; \chi_{m\epsilon_M}(x)\; \phi(x), \qquad \pi_M(m) := (E_M\pi)(m) := \pi(m\epsilon_M) \tag{III.85}$$

Notice that (III.85) defines a partial symplectomorphism

$$\{\pi_M(m), \phi_M(m')\} = \int d^Dx \; \chi_{m\epsilon_M}(x)\; \{\pi(x), \phi(m'\epsilon_M)\} = \chi_{m\epsilon_M}(m'\epsilon_M) = \delta_{mm'} \tag{III.86}$$

The Hamiltonian (II.166) gets hence identified with following discretised family

$$H_M^{(0)} := \frac{c}{2} \sum_{m\in\mathbb{Z}_M^D} (\kappa_\phi \epsilon_M^D \pi_M^2(m) + \frac{1}{\kappa_\phi \epsilon_M^D} \phi_M(m)[(\omega_M^{(0)})^2 \cdot \phi_M](m)) \tag{III.87}$$

Here we have defined $\omega_M^{(0)}$ in terms of a suitable, self-adjoint (with respect to L_M) discretisation Δ_M of the Laplacian, that is, if the continuum ω is a certain function $G = G(-\Delta_R, p^2)$ of the continuum Laplacian Δ_R on $[0,R)^D$ then $\omega_M^{(0)}$ is the function $G(-\Delta_M, p^2)$.
It is not difficult to check that (III.87) converges to

$$H := \frac{c}{2} \int_{[0,R)^D} d^Dx \; [\kappa_\phi \pi^2 + \frac{1}{\kappa_\phi} \phi \omega_R^2 \phi] \tag{III.88}$$

on smooth fields as $M \to \infty$.

The form (III.87) of the Hamiltonian motivates to follow the strategy of (II.167) and introduce discrete annihilation functions

$$a_M^{(0)} := \frac{1}{\sqrt{2\hbar\kappa_\phi}} [\sqrt{\frac{\omega_M^{(0)}}{\epsilon_M^D}} \phi_M - i\kappa_\phi \sqrt{\frac{\epsilon_M^D}{\omega_M^{(0)}}} \pi_M] \tag{III.89}$$

so that upon choosing them as the non-commutative algebra of observables we introduce the ordering

$$H_M^{(0)} = \hbar c \sum_{m\in\mathbb{Z}_M^D} (a_M^{(0)})^* \, \omega_M^{(0)} \cdot a_M^{(0)} \tag{III.90}$$

The quantisation of this system is now analogous to the quantisation of finitely many harmonic oscillators and hence well understood. By promoting $a_M^{(0)}$ to the annihilation operators $\hat{a}_M^{(0)}$ we introduce the vacuum $\Omega_M^{(0)}$ with the property $a_M^{(0)}(m)\Omega_M^{(0)} = 0, \ \forall m \in \mathbb{Z}_M^D$. Consequently $\hat{H}\Omega_M^{(0)} = 0$. The corresponding Hilbert space spanned by the polynomials of $\hat{a}_M^*(m)$ acting on the vacuum is found to be $L_2(\mathbb{R}^{M^D}, d\nu_M^{(0)})$. We choose the ground state representation $\Omega_M = 1$ and find up to normalisation (compare to (II.215))

$$\begin{aligned} d\nu_M^{(0)}(\phi_M) \ &= \ \exp(\hbar\kappa_\phi \langle \phi_M(\omega_M^{(0)})\phi_M\rangle_M) \ d\phi_M^{M^D} \ , \Rightarrow \\ &\nu_M^{(0)}(e^{i\phi_M[f_M]}) = e^{-\frac{1}{2}\langle f_M, c_M f_M\rangle_M} \end{aligned} \tag{III.91}$$

where we will call $c_M = \hbar\kappa_\phi 2\omega_M^{(0)}$ the *covariance*. Hence, we have constructed explicitly a family of OS data $(\mathcal{H}_{RM}^{(0)}, H_{RM}^{(0)}, \Omega_{RM}^{(0)})$ which certainly is not a fixed point family.

We sidestep the introduction of a temporal cut-off T and its corresponding temporal renormalisation and directly construct the Wiener measure family $\mu_M^{(0)}$ on the history spaces Γ_M of fields Φ_M corresponding to the OS data constructed above. The construction is entirely identical to the continuum calculation, hence we know that the Wiener measure family $\mu_M^{(0)}$ is described by a Gaussian measure with the covariance

$$C_M^{(0)} = \frac{\hbar\kappa_\phi}{2}(-\frac{1}{c^2}\partial_t^2 + [\omega_M^{(0)}]^2) \tag{III.92}$$

We set c=1 in the following subsections and restrict our attention to the case $D = 1$. The generalisation to more dimension will be undergone in the section III.E.

III.C.1 Flow of the PI induced Hamiltonian Renormalisation

Following the general programme, the first step in [129] was to calculate the flow of the sequence of measure families $\mu_M^{(0)}$ and its fixed point. As we follow them closely, we consider the maps $I_{M\to 2M}$ which is an isometric injection,

$$\begin{aligned} \langle I_{M\to 2M} \cdot f_M, I_{M\to 2M} \cdot f'_M \rangle_{L_{2M}} &= \langle I_{2M} \circ I_{M\to 2M} \cdot f_M, I_{2M} \circ I_{M\to 2M} \cdot f'_M \rangle_{L_R} \\ &= \langle I_M \cdot f_M, I_M \cdot f'_M \rangle_{L_R} = \langle f_M, f'_M \rangle_{L_M} \end{aligned} \tag{III.93}$$

where we used the isometry of I_M and (III.18). Explicitly for $m \in \mathbb{Z}_{2M}^D$

$$[I_{M\to 2M} \cdot f_M](m) = \sum_{m'\in\mathbb{Z}_M^D} \chi_{m'\epsilon_M}(m\epsilon_{2M}) f_M(m') = f_M(\lfloor m/2 \rfloor) \tag{III.94}$$

where $\lfloor m/2 \rfloor^a := \lfloor m^a/2 \rfloor, \ a = 1,..,D$ denotes the component wise Gauss bracket.

The path integral flow is defined by

$$\mu_M^{(n+1)}(e^{i\Phi_M[F_M]}) := \mu_{2M}^{(n)}(e^{i\Phi_{2M}[I_{M\to 2M}F_M]}) \tag{III.95}$$

and it follows immediately that the flow generates a family of Gaussian measures with covariances $C_M^{(n)}$ since the initial family is such. Namely we find[10]

$$C_M^{(n+1)} = (\mathbb{1}_{L_2} \otimes I_{M\to 2M})^\dagger \ C_{2M}^{(n)} \ (\mathbb{1}_{L_2} \otimes I_{M\to 2M}) \tag{III.96}$$

where the notation is to indicate, that no temporal renormalisation takes place.

In the continuum the kernel of the covariance is defined as

$$\langle F, C_R \cdot F \rangle_{L_2 \otimes L_R} =: \int_{\mathbb{R}^2} ds \ ds' \int_{[0,R)^{2D}} d^Dx \ d^Dy \ F(s,x) \ C_R((s,x),(s',y)) \ F(s',y) \tag{III.97}$$

[10] Note that this simple consequence, i.e. the new measure is again of Gaussian nature with changed covariance, is the crucial point due to which the renormalisation can be carried out analytically. In general, the nature of the measure itself can change drastically and such an easy relation may no longer be valid.

It follows

$$
\begin{aligned}
& \langle 1_{L_2} \otimes I_M \cdot F_M, C_R \cdot 1_{L_2} \otimes I_M \cdot F_M \rangle_{L_2 \otimes L_R} = \\
= \quad & \langle F_M, [(1_{L_2} \otimes I_M)^\dagger C_R (1_{L_2} \otimes I_M)] F_M \rangle_{L_2 \otimes L_M} =: \langle F_M, C_M F_M \rangle_{L_M}
\end{aligned} \tag{III.98}
$$

which shows that

$$
C_M((s,m),(s',m')) = \epsilon_M^{-2D} \langle \chi_{m\epsilon_M}, C_R((s,.),(s',.)) \chi_{m'\epsilon_M} \rangle_{L_R} \tag{III.99}
$$

Note that the continuum kernel family is automatically a fixed point of (III.96) due to $I_M = I_{2M} \circ I_{M \to 2M}$. Expression (III.99) tends to $C_R((s, m\epsilon_M), (s', m'\epsilon_M))$ as $M \to \infty$.

Explicitly, we have in terms of the kernel of the covariance for the flow of the discretised covariance

$$
\begin{aligned}
& \langle F_M, C_M^{(n+1)} F_M \rangle_{L_2 \otimes L_M} = \epsilon_M^{2D} \sum_{m_1', m_2' \in \mathbb{Z}_M^D} \int ds ds' \; F_M(s, m_1') F_M(s', m_2') C_M^{(n+1)}((s, m_1'), (s', m_2')) \\
& = \langle (1_{L_2} \otimes I_{M \to 2M}) \cdot F_M, C_{2M}^{(n)} (1_{L_2} \otimes I_{M \to 2M}) \cdot F_M \rangle_{L_2 \otimes L_{R2M}} \\
& = \epsilon_{2M}^{2D} \sum_{m_1, m_2} \int ds ds' \; (1_{L_2} \otimes I_{M \to 2M} \cdot F_M)(s, m_1)(1_{L_2} \otimes I_{M \to 2M} \cdot F_M)(s', m_2) C_{2M}^{(n)}((s, m_1), (s', m_2)) \\
& = \frac{\epsilon_M^{2D}}{2^{2D}} \int ds ds' \sum_{m_1, m_2 \in \mathbb{Z}_{2M}^D} F_M(s, \lfloor m_1/2 \rfloor) F_M(s', \lfloor m_2/2 \rfloor) C_{2M}^{(n)}((s, m_1), (s', m_2)) \\
& = \frac{\epsilon_M^{2D}}{2^{2D}} \sum_{m_1', m_2' \in \mathbb{Z}_M^D} \int ds ds' \; F_M(s, m_1') F_M(s', m_2') \sum_{\lfloor m_1/2 \rfloor = m_1', \lfloor m_2/2 \rfloor = m_2'} C_{2M}^{(n)}((s, m_1), (s', m_2))
\end{aligned} \tag{III.100}
$$

from which we read off that for all F_M:

$$
C_M^{(n+1)}((s, m_1'), (s', m_2')) = 2^{-2D} \sum_{\delta_1, \delta_2 \in \{0,1\}^D} C_{2M}^{(n)}((s, 2m_1' + \delta_1), (s', 2m_2' + \delta_2)) \tag{III.101}
$$

This condition describes the renormalisation flow and deducing its corresponding fixed point gives us the Gaussian measure of the continuum theory restricted to spatially coarse observables.

A simplification can be achieved by making use of the translation invariance of the (discrete) Laplacian and thus the corresponding covariances $C_M((s,m),(s',m')) = C_M(s-s', m-m')$, a property which is preserved by inspection under the block spin transformation (III.101). This suggests using Fourier transform techniques. Recall that L_R is equipped with the orthonormal basis $R^{-D/2} e^{ik_R n \cdot x}$, $n \in \mathbb{Z}^D$, $x \in [0, R)^D$ where $k_R = \frac{2\pi}{R}$. If we restrict x to the lattice points $x = m\epsilon_M$, $m \in \mathbb{Z}_M^D$ then $e^{ik_R n \cdot x} = e^{ik_M n \cdot m}$, $k_M = \frac{2\pi}{M}$ and we may restrict n to $\mathbb{Z}_M^D$ as well, due to periodicity of the argument of the exponential function. Indeed, we may define Fourier transform and its inverse on L_M by

$$
f_M(m) =: \sum_{n \in \mathbb{Z}_M^D} \hat{f}_M(n) \, e^{ik_M n \cdot m}, \qquad \hat{f}_M(n) =: M^{-D} \sum_{m \in \mathbb{Z}_M^D} f_M(m) \, e^{-ik_M n \cdot m} \tag{III.102}
$$

The discrete Fourier transform has the advantage that it diagonalises the Laplacian $[\Delta_M e^{ik_M n \cdot}](m) = -\hat{\Delta}_M(k_M n) e^{ik_M n \cdot m}$ with $\hat{\Delta}_M(k_M n) \in \mathbb{R}$. And if $C_M^{(n)} = G(-\partial_t^2, -\Delta_M, p^2)$ then we have

$$
\begin{aligned}
& [C_M^{(n)} \cdot F_M](s, m) = \epsilon_M^D \sum_{m' \in \mathbb{Z}_M^D} \int ds' \; C_M^{(n)}(s - s', m - m') F_M(s', m') \\
& = \sum_{n \in \mathbb{Z}_M^D} \int \frac{dk_0}{2\pi} \; \hat{F}_M(k_0, n) \, G(k_0^2, -\hat{\Delta}_M(nk_M), p^2) \, e^{i(k_0(s-s') + k_M n \cdot (m - m'))} \\
& = \sum_{m' \in \mathbb{Z}_M^D} \int ds' \; F_M(s', m') [M^{-D} \sum_{n \in \mathbb{Z}_M^D} \int \frac{dk_0}{2\pi} e^{i(k_0(s-s') + k_M n \cdot (m - m'))} G(k_0^2, -\hat{\Delta}_{RM}(nk_M), p^2)]
\end{aligned} \tag{III.103}
$$

If we define $\hat{C}_M^{(n)}(k_0, n) := R^{-D} G(k_0^2, -\hat{\Delta}_M(k_M n), p^2)$ we find:

$$
C_M^{(n)}(s - s', m - m') = \sum_{n \in \mathbb{Z}_M^D} \int \frac{dk_0}{2\pi} \; e^{i(k_0(s-s') + k_M n \cdot (m - m'))} \hat{C}_M^{(n)}(k_0, n) \tag{III.104}
$$

for the discretised family.

Since for general ω_R it is explicitly only possible to study the flow of the covariance in terms of its Fourier transform we translate (III.101) in terms of the Fourier transform

$$C_M^{(n+1)}((s,m_1'),(s',m_2')) = \sum_{l'\in\mathbb{Z}_M^D} \int \frac{dk_0}{2\pi}\, e^{i(k_0(s-s')+k_M l'\cdot(m-m'))}\, \hat{C}_M^{(n+1)}(k_0,l') \tag{III.105}$$

$$= 2^{-2D} \sum_{l\in\mathbb{Z}_{2M}^D} \int \frac{dk_0}{2\pi}\, \hat{C}_{2M}^{(n)}(k_0,l) \sum_{\delta_1,\delta_2\in\{0,1\}^D} e^{i(k_0(s-s')+k_{2M} l\cdot(2(m_1'-m_2')+\delta_1-\delta_2))}$$

$$= 2^{-2D} \sum_{l'\in\mathbb{Z}_M^D} \int \frac{dk_0}{2\pi} \sum_{\delta_1,\delta_2,\delta_3\in\{0,1\}^D} \hat{C}_{2M}^{(n)}(k_0,l'+\delta_3 M) e^{i(k_0(s-s')+k_{2M}(l'+\delta_3 M)\cdot(2(m_1'-m_2')+\delta_1-\delta_2))}$$

$$= 2^{-2D} \sum_{l'\in\mathbb{Z}_M^D} e^{ik_M l'\cdot(m_1'-m_2')} \int \frac{dk_0}{2\pi} \sum_{\delta_1,\delta_2,\delta_3\in\{0,1\}^D} \hat{C}_{2M}^{(n)}(l'+\delta_3 M) e^{i(k_0(s-s')+k_{2M}(l'+\delta_3 M)\cdot(\delta_1-\delta_2))}$$

whence

$$\hat{C}_M^{(n+1)}(k_0,l') = 2^{-2D} \sum_{\delta_1,\delta_2,\delta_3\in\{0,1\}^D} \hat{C}_{2M}^{(n)}(k_0,l'+\delta_3 M) e^{ik_{2M}(l'+\delta_3 M)\cdot(\delta_1-\delta_2)} \tag{III.106}$$

We will now carry out the details of this procedure for illustrative purposes for the case $D=1$ and the Poincaré invariant choice

$$\omega_R = \sqrt{-\Delta_R + p^2} \tag{III.107}$$

More general models in all dimensions will be discussed in the last section of this chapter III.E. For $D=1$ (III.106) becomes with $l'\in\mathbb{Z}_M$

$$\begin{aligned}\hat{C}_M^{(n+1)}(k_0,l') &= \frac{1}{2}\sum_{\delta_3\in\{0,1\}} \hat{C}_{2M}^{(n)}(k_0,l'+\delta_3 M)[1+\cos(k_{2M}(l'+\delta_3 M))] \\ &= \frac{1}{2}\{\hat{C}_{2M}^{(n)}(k_0,l')[1+\cos(k_{2M}l')] + \hat{C}_{2M}^{(n)}(k_0,l'+M)[1-\cos(k_{2M}l')]\}\end{aligned} \tag{III.108}$$

We start the flow with $\hat{C}_M^{(0)}(k_0,l') := \hat{C}_M(k_0,l')$ where $C_M(k_0,l')$ corresponds to a naive discretisation of the Laplacian. For it, we take a popular choice in $D=1$:

$$(\Delta_M\cdot f_M)(m) := \frac{1}{\epsilon_M^2}[f_M(m+1)+f_M(m-1)-2f_M(m)] \tag{III.109}$$

Going over to Fourier picture, we see that

$$-\hat{\Delta}_M(l)e^{ik_M n\cdot l} = (\Delta_M e^{ik_M n\cdot})(l) = \epsilon_M^{-2}(e^{ik_M n(l+1)} + e^{ik_M n(l-1)} - 2e^{ik_M nl}) = 2\epsilon_M^{-2}(\cos(k_M n)-1)e^{ik_M nl}$$

Thus, from (III.92) and (III.104) with $l\in\mathbb{Z}_M$

$$\hat{C}_M^{(0)}(k_0,l) = R^{-1}\frac{\hbar\kappa_\phi}{2}\frac{1}{2\epsilon_M^{-2}[1-\cos(k_M l)]+k_0^2+p^2} \tag{III.110}$$

It is equivalent to study the flow of $\hat{c}_M(l) := 2R\hat{C}_M(l)/(\hbar\kappa_\phi)$ and it is convenient to introduce the abbreviations $t := k_M l, q := \sqrt{k_0^2+p^2}\epsilon_M$. Hence

$$\hat{c}_M^{(0)}(l) = \frac{\epsilon_M^2}{2[1-\cos(t)]+q^2} \tag{III.111}$$

For reasons that will become transparent in a moment we rewrite (III.111) as follows: Let

$$a_0(q) := 1+q^2/2,\ b_0(q) := q^3/2, c_0(q) := 0 \tag{III.112}$$

then trivially

$$\hat{c}_M^{(0)}(l) = \frac{\epsilon_M^2}{q^3}\,\frac{b_0(q)+c_0(q)\cos(t)}{a_0(q)-\cos(t)} \tag{III.113}$$

The purpose of doing this trivial rewriting is that it turns out that the parametrisation by 3 functions a_n, b_n, c_n of q in the Ansatz

$$\hat{c}_M^{(n)}(l) = \frac{\epsilon_M^2}{q^3}\,\frac{b_n(q)+c_n(q)\cos(t)}{a_n(q)-\cos(t)} \tag{III.114}$$

is invariant under the renormalisation flow. Namely, by (III.108) (note $t = k_M l \to k_{2M} l = t/2, q = \sqrt{k_0^2+p^2}\epsilon_M \to \sqrt{k_0^2+p^2}\epsilon_{2M} = q/2$ and $\cos(k_{2M}(l+M)) = -\cos(t/2)$)

$$\begin{aligned}
\hat{c}_M^{(n+1)}(l) &= \frac{\epsilon_M^2}{q^3}\,\frac{b_{n+1}(q)+c_{n+1}(q)\cos(t)}{a_{n+1}(q)-\cos(t)} \qquad \text{(III.115)}\\
&= \frac{1}{2}\{\hat{c}_{2M}^{(n)}(l)[1+\cos(k_{2M}l)] + \hat{c}_{2M}^{(n)}(l+M)[1-\cos(k_{2M}l)]\}\\
&= \frac{\epsilon_{2M}^2}{2(q/2)^3}\{\frac{b_n(q/2)+c_n(q/2)\cos(t/2)}{a_n(q/2)-\cos(t/2)}[1+\cos(t/2)] + \frac{b_n(q/2)-c_n(q/2)\cos(t/2)}{a_n(q/2)+\cos(t/2)}[1-\cos(t/2)]\}\\
&= \frac{\epsilon_M^2}{q^3}\frac{1}{a_n(q/2)^2-\cos^2(t/2)}\{[b_n(q/2)+c_n(q/2)\cos(t/2)][a_n(q/2)+\cos(t/2)][1+\cos(t/2)]\\
&\quad +[b_n(q/2)-c_n(q/2)\cos(t/2)][a_n(q/2)-\cos(t/2)][1-\cos(t/2)]\}\\
&= \frac{\epsilon_M^2}{q^3}\frac{1}{a_n(q/2)^2-\frac{1}{2}[1+\cos(t)]}\{2a_n(q/2)b_n(q/2) + 2\cos^2(t/2)[b_n(q/2)+c_n(q/2)+a_n(q/2)c_n(q/2)]\}\\
&= \frac{\epsilon_M^2}{q^3}\frac{1}{[2a_n(q/2)^2-1]-\cos(t)}\{2[2a_nb_n+b_n+c_n+a_nc_n](q/2) + 2[b_n+c_n+a_nc_n](q/2)\cos(t)\}
\end{aligned}$$

where we used the double-angle relation: $2\cos(t/2)^2 = 1+\cos(t)$. We deduce the recursion relations

$$\begin{aligned}
a_{n+1}(q) &= 2a_n(q/2)^2-1\\
b_{n+1}(q) &= 2[2a_nb_n+b_n+c_n+a_nc_n](q/2)\\
c_{n+1}(q) &= 2[b_n+c_n+a_nc_n](q/2)
\end{aligned} \tag{III.116}$$

The corresponding fixed point equations become coupled functional equations

$$\begin{aligned}
a_*(q) &= 2a_*(q/2)^2-1\\
b_*(q) &= 2[2a_*b_*+b_*+c_*+a_*c_*](q/2)\\
c_*(q) &= 2[b_*+c_*+a_*c_*](q/2)
\end{aligned}$$

The easiest of these three equations is the first one, as it involves only one function and we easily recognise the functional equation of the cosine or hyperbolic cosine. Now, $a_0(q) > 1$ for $q > 0$ and assuming this to be the case also for $a_n(q)$ we get $a_{n+1}(q) = 2a_n(q/2)^2 - 1 > 1$ for $q > 0$. It follows $a_*(q) > 1$ for $q > 0$ so that

$$a_*(q) = \mathrm{ch}(q) \tag{III.117}$$

Next we observe

$$d_*(q) := (b_*+c_*)(q) = 4[1+a_*(q/2)][b_*+c_*](q/2) \tag{III.118}$$

which is a homogeneous linear functional equation as a_* is already known. If we define $[b_*+c_*](q) = q^n P(\mathrm{ch}(q))$ where P is a polynomial then we have a chance to satisfy the fixed point equation since q^n can take the factor of 4 into account and the right hand side depends only on $\mathrm{ch}(q/2)$ as well as the left hand side. To see this, remember that $\mathrm{ch}(q) = 2\mathrm{ch}^2(q/2) - 1$.
Let $P = \sum_{k=0}^N z_k \mathrm{ch}^k(q)$, then in terms of $x = \mathrm{ch}(q/2)$ the fixed point condition becomes

$$2^n \sum_{k=0}^N z_k[2x^2-1]^k = 4(x+1)\sum_{k=0}^N z_k x^k = 4\{z_0 + z_N x^{N+1} + \sum_{k=1}^N [z_k+z_{k-1}]x^k\} \tag{III.119}$$

We may assume that $z_N \neq 0$, otherwise decrease the degree of the polynomial. Then we must have $2N = N+1$ i.e. $N = 1$. It follows

$$2^n\{z_0 - z_1 + 2z_1x^2\} = 4\{z_0 + (z_0+z_1)x + z_1x^2\} \tag{III.120}$$

i.e.

$$n = 1,\ z_1 = -z_0 \ \Rightarrow\ zq(\mathrm{ch}(q)-1) =: d_*(q) \tag{III.121}$$

where z is a constant to be determined later.

Finally we have

$$c_*(q) = 2(b_* + c_*)(q/2) + 2a_*(q/2)c_*(q/2) = 2d_*(q/2) + 2a_*(q/2)c_*(q/2) \tag{III.122}$$

which is an inhomogeneous linear functional equation as a_*, d_* are already known. The general solution will therefore be the linear combination of a special solution c_1 of the inhomogeneous equation and the general solution c_2 of the corresponding homogeneous equation. Explicitly

$$0 = -c_1(q) + zq(\text{ch}(q/2) - 1) + 2\text{ch}(q/2)c_1(q/2) = -[c_1(q) + zq] + \text{ch}(q/2)[2c_1(q/2) + zq] \tag{III.123}$$

which is solved by $c_1(q) = -zq$. This leaves us with

$$c_2(q) = 2\text{ch}(q/2)c_2(q/2) \tag{III.124}$$

which is the functional equation of $c_2(q) = z'\text{sh}(q)$ where again z' is a constant to be determined later. In total this means

$$c_*(q) = z'\text{sh}(q) - zq \tag{III.125}$$

To see which values z, z' are chosen by the initial functions of the fixed point equation we notice that $d_0(q) = q^3/2$ and assume $\lim_{q\to 0} 2d_n(q)/q^3 = 1$ up to some n then also

$$\lim_{q\to 0} \frac{2d_{n+1}(q)}{q^3} = \lim_{q\to 0} \frac{8[\text{ch}(q/2)+1]d_n(q/2)}{q^3} = \lim_{q\to 0} \frac{2d_n(q/2)}{(q/2)^3} = 1 \tag{III.126}$$

Thus also $\lim_{q\to 0} 2d_*(q)/q^3 = 1$ whence $z = 1$. Finally we have $c_0(q) = 0$ hence $\lim_{q\to 0} c_0(q)/q^3$ regular. We assume this to be the case up to some n i.e. $c_n(q) = O(q^3)$. Then

$$c_{n+1}(q)/q^3 = 2d_n(q/2)/q^3 + 2a_n(q/2)c_n(q/2)/q^3 \tag{III.127}$$

is also regular at $q = 0$ hence so must be $c_*(q)$. It follows $z' = 1$.

We summarise: The fixed point equation is uniquely solved by

$$\begin{aligned} a_*(q) &= \text{ch}(q) \\ b_*(q) &= q\text{ch}(q) - \text{sh}(q) \\ c_*(q) &= \text{sh}(q) - q \end{aligned} \tag{III.128}$$

III.C.2 Comparison to the Continuum

We now compare this to the cylindrical projections of the known continuum theory. As those have been computed first in [129] we quote their calculations.

The continuum theory is described by the covariance $C_R = \frac{\hbar\kappa_\phi}{2}(-\partial_t^2 - \Delta_R + p^2)^{-1}$ or equivalently $c_R = \frac{2R}{\hbar\kappa_\phi} C_R = R(-\partial_t^2 - \Delta_R + p^2)^{-1}$ which can now be directly compared to (III.111). The corresponding cylindrical projection at resolution M is

$$\begin{aligned} c_M((s,m),(s',m')) &= \epsilon_M^{-2}([\mathbb{1}_{L_2} \otimes I_M]^\dagger c_R [\mathbb{1}_{L_2} \otimes I_M])((s,m),(s',m')) \\ &= \epsilon_M^{-2} \int_{m\epsilon_M}^{(m+1)\epsilon_M} dx \int_{m'\epsilon_M}^{(m'+1)\epsilon_M} dy\; c_R((s,x),(s',y)) \end{aligned} \tag{III.129}$$

where $c_R(x,y)$ is the continuum kernel. To compute it, we employ again Fourier transformation and use the fact that the functions $e_{nR}(x) = e^{ink_R x}/\sqrt{R},\ k_R = 2\pi/R$ form an orthonormal basis on $L_R = L_2([0,R), dx)$. Hence

$$\begin{aligned} c_R((s,x),(s',y)) &= R(-\partial_s^2 - \Delta_{Rx} + p^2)^{-1}\delta_{\mathbb{R}}(s,s')\delta_R(x,y) \qquad \text{(III.130)} \\ &= \int \frac{dk_0}{2\pi} \sum_{n\in\mathbb{Z}} e_{-nR}(y)\; R(-\partial_s^2 - \Delta_{Rx} + p^2)^{-1} e^{ik_0(s-s')}\; e_{nR}(x) \\ &= \int \frac{dk_0}{2\pi} \sum_{n\in\mathbb{Z}} \frac{e^{i(k_0(s-s') + k_R n(x-y))}}{(nk_R)^2 + k_0^2 + p^2} \end{aligned}$$

It follows

$$
\begin{aligned}
&c_M((s,m),(s',m')) = \qquad \text{(III.131)}\\
&= \epsilon_M^{-2}\sum_{n\in\mathbb{Z}}\int \frac{dk_0}{2\pi}\;\frac{e^{ik_0(s-s')}}{(nk_R)^2+k_0^2+p^2}\;[\int_{m\epsilon_M}^{(m+1)\epsilon_M} dx\; e^{ik_Rnx}][\int_{m'\epsilon_M}^{(m'+1)\epsilon_M} dy\; e^{-ik_Rny}]\\
&= \epsilon_M^{-2}\sum_{n\in\mathbb{Z}}\int \frac{dk_0}{2\pi}\;\frac{e^{ik_0(s-s')}}{(nk_R)^2+k_0^2+p^2}\;[\epsilon_M\delta_{n,0}+\frac{1-\delta_{n,0}}{ik_Rn}(e^{ik_Rn(m+1)\epsilon_M}-e^{ik_Rnm\epsilon_M})]\times\\
&\qquad\times[\epsilon_M\delta_{n,0}-\frac{1-\delta_{n,0}}{ik_Rn}(e^{-ik_Rn(m'+1)\epsilon_M}-e^{-ik_Rnm'\epsilon_M})]\\
&= \sum_{n\in\mathbb{Z}}\int \frac{dk_0}{2\pi}\;\frac{e^{i(k_0(s-s')+k_Mn(m-m')}}{(nk_R)^2+k_0^2+p^2}\;[\delta_{n,0}+2\frac{1-\delta_{n,0}}{(k_Mn)^2}(1-\cos(k_Mn)]
\end{aligned}
$$

To compare this expression to $\hat{c}_M(k_0,l),\ l\in\mathbb{Z}_M$ we write $n=l+NM,\ N\in\mathbb{Z}$ and split the sum

$$
c_M((s,m),(s',m')) = \sum_{l\in\mathbb{Z}_M}\int\frac{dk_0}{2\pi}\sum_{N\in\mathbb{Z}}\frac{e^{i(k_0(s-s')+k_Ml(m-m'))}}{([l+NM]k_R)^2+k_0^2+p^2}\;\frac{2(1-\cos([l+NM]k_M))}{([l+NM]k_M)^2} \tag{III.132}
$$

where we declare the last fraction to equal unity at $l=N=0$. Comparing with the first line of (III.105) we see that the sum involved in (III.105) coincides with the definition of $\hat{c}_M(k_0,l)$.

We now carry out the sum over N by employing the Poisson summation formula

Theorem III.C.1 (Poisson Summation Formula). *Consider $f\in L_1(\mathbb{R},dx)$ such that the series $\sum_{n\in\mathbb{Z}} f(y+ns)$ is absolutely and uniformly convergent for $y\in[0,s],\ s>0$. Then*

$$
\sum_{n\in\mathbb{Z}} f(ns) = \sum_{n\in\mathbb{Z}}\int_{\mathbb{R}} dx\cdot e^{-i2\pi nx} f(sx) \tag{III.133}
$$

Beweis. See e.g. the book about Fourier analysis by Bochner [214]. □

In our case we choose

$$
f(x) := \frac{1}{([l+xM]k_R)^2+k_0^2+p^2}\;\frac{2(1-\cos([l+xM]k_M)}{([l+xM]k_M)^2} \tag{III.134}
$$

to which the Poisson resummation may be applied as f is smooth and decays at infinity as $1/x^4$. We find with $q=\sqrt{k_0^2+p^2}\epsilon_M$

$$
\begin{aligned}
\hat{c}_M^\infty(k_0,l) &= \sum_{N\in\mathbb{Z}}\frac{1}{([l+NM]k_R)^2+k_0^2+p^2}\;\frac{2(1-\cos([l+NM]k_M))}{([l+NM]k_M)^2}\\
&= \epsilon_M^2\sum_{N\in\mathbb{Z}}\int dx\; e^{-i2\pi Nx}\;\frac{1}{([l+xM]k_M)^2+q^2}\;\frac{2(1-\cos([l+xM]k_M))}{([l+xM]k_M)^2}\\
&= \epsilon_M^2\sum_{N\in\mathbb{Z}}\int dx\; e^{-i2\pi Nx}\;\frac{1}{(k_Ml+2\pi x)^2+q^2}\;\frac{2(1-\cos(k_Ml+2\pi x))}{(k_Ml+2\pi x)^2}\\
&= \epsilon_M^2\sum_{N\in\mathbb{Z}}\int \frac{dx}{2\pi}\; e^{-iNx}\;\frac{1}{(k_Ml+x)^2+q^2}\;\frac{2(1-\cos(k_Ml+x))}{(k_Ml+x)^2}\\
&= \epsilon_M^2\sum_{N\in\mathbb{Z}} e^{ik_MNl}\int\frac{dx}{2\pi}\;\frac{2e^{-iNx}(1-\cos(x))}{x^2(x^2+q^2)}
\end{aligned} \tag{III.135}
$$

We have

$$
\frac{2(1-\cos(x))e^{-iNx}}{x^2} = \frac{e^{-iNx}-e^{-i(N-1)x}}{x^2}+\frac{e^{-iNx}-e^{-i(N+1)x}}{x^2} \tag{III.136}
$$

For any N (III.136) is holomorphic in the entire complex plane and for $N\geq 1$ decays on the lower infinite half-circle and for $N\leq -1$ decays on the upper infinite half-circle. It follows that the integrand is holomorphic everywhere in the whole complex plane except at $x=\pm iq$ and the contour can be closed as described for $N\neq 0$. Thus we find by the residue theorem

$$
\int\frac{dx}{2\pi}\;\frac{2e^{-iNx}(1-\cos(x))}{x^2(x^2+q^2)} = \begin{cases} -\frac{2\pi i}{2\pi}\frac{2e^{-iNx}(1-\cos(x))}{x^2(x-iq)}\Big|_{x=-iq} & N\geq 1\\ \frac{2\pi i}{2\pi}\frac{2e^{-iNx}(1-\cos(x))}{x^2(x+iq)}\Big|_{x=iq} & N\leq -1\end{cases} = \frac{e^{-|N|q}(\mathrm{ch}(q)-1)}{q^3} \tag{III.137}
$$

For $N=0$ the first term in (III.136) decays on the upper while the second decays on the lower infinite half circle. However, the two terms are not separately holomorphic at $x=0$, only their sum is. We thus write the integral as a principal value integral $\lim_\delta \to 0$ where we leave out the interval $[-\delta,\delta]$ and then close the contour for the first/second term with a small half-circle of radius δ in the upper/lower complex plane, subtract that added contribution and apply the residue theorem. We find

$$\begin{aligned}\int \frac{dx}{2\pi}\,\frac{2(1-\cos(x))}{x^2(x^2+q^2)^2} &= -\frac{2\pi i}{2\pi}\frac{(1-e^{-ix})}{x^2(x-iq)}_{x=-iq} - \lim_{\delta\to 0}\int_{x=\delta e^{i\phi},\,\phi\in[-\pi,0]}\frac{dx}{2\pi x}\,\frac{1-e^{-ix}}{x}\,\frac{1}{x^2+q^2}\\ &\quad +\frac{2\pi i}{2\pi}\frac{(1-e^{ix})}{x^2(x+iq)}_{x=iq} + \lim_{\delta\to 0}\int_{x=\delta e^{i\phi},\,\phi\in[0,\pi]}\frac{dx}{2\pi x}\,\frac{1-e^{ix}}{x}\,\frac{1}{x^2+q^2}\\ &= \frac{q+e^{-q}-1}{q^3} \end{aligned} \tag{III.138}$$

It remains to compute the geometric sum in (III.135) with $k_M l = t$

$$\begin{aligned}\frac{\hat{c}_M(l)}{\epsilon_M^2} &= \frac{q+e^{-q}-1}{q^3}+\frac{\mathrm{ch}(q)-1}{q^3}(-2+\sum_{N=0}^{\infty}\{e^{-N[q+it]}+e^{-N[q-it]}\})\\ &= \frac{q+e^{-q}-1-\mathrm{ch}(q)+1}{q^3}+\frac{\mathrm{ch}(q)-1}{q^3}(-1+\frac{1}{1-e^{-[q+it]}}+\frac{1}{1-e^{-[q-it]}})\\ &= \frac{q-\mathrm{sh}(q)}{q^3}+\frac{\mathrm{ch}(q)-1}{q^3}\,\frac{2-2e^{-q}\cos(t)-[1+e^{-2q}-2e^{-q}\cos(t)]}{1+e^{-2q}-2e^{-q}\cos(t)}\\ &= \frac{q-\mathrm{sh}(q)}{q^3}+\frac{\mathrm{ch}(q)-1}{q^3}\,\frac{\mathrm{sh}(q)}{\mathrm{ch}(q)-\cos(t)}\\ &= \frac{1}{q^3}\,\frac{1}{\mathrm{ch}(q)-\cos(t)}\,\{[\mathrm{ch}(q)-1]\mathrm{sh}(q)+[q-\mathrm{sh}(q)]\mathrm{ch}(q)-[q-\mathrm{sh}(q)]\cos(t)\}\\ &= \frac{1}{q^3}\,\frac{1}{\mathrm{ch}(q)-\cos(t)}\,\{[q\mathrm{ch}(q)-\mathrm{sh}(q)]+[\mathrm{sh}(q)-q]\cos(t)\} \end{aligned} \tag{III.139}$$

Comparing with (III.114) and (III.128) we see that we obtain *perfect match*! The fixed point equations of the naively discretised covariance of the history field measure have found the *precise* cylindrical projections of its continuum covariance $[-\partial_t^2-\Delta_R+p^2]^{-1}$. It is therefore clear that the fixed point path integral precisely delivers the continuum OS data via OS reconstruction that we started from and that we artificially discretised. Moreover, it is easy to see that the continuum limit $\lim_{M\to\infty} c_M(l)=[k_0^2+m^2+(lk_R)^2]^{-1}$ coincides with the continuum covariance.

III.C.3 Matrix elements of the Hamiltonian from PI induced Renormalisation

We carry out the explicit OS reconstruction of the measures $\mu_R^{(n)}$. This is taken from [129]. To do this recall that these are determined by the covariances of their Fourier transform which up to a factor follow the flow ($l\in\mathbb{Z}_M$), see (III.108)

$$\begin{aligned}\hat{c}_M^{(n+1)}(k_0,l) &= \frac{1}{2}\{\hat{c}_{2M}^{(n)}(k_0,l)[1+\cos(t/2)]+\hat{c}_{2M}^{(n)}(k_0,l+M)[1-\cos(t/2)]\},\\ \hat{c}_M^{(0)}(k_0,l) &= \frac{\epsilon_M^2}{2[1-\cos(t)]+q^2},\; t=k_M l, q=\sqrt{p^2+k_0^2}\epsilon_M \end{aligned} \tag{III.140}$$

We conclude that while $c_M^{(0)}(k_0,l)$ displays only one simple pole with respect to q^2, the number of poles gets doubled at each renormalisation step. For instance

$$\hat{c}_M^{(1)}(k_0,l)=\frac{\epsilon_M^2}{8}\{\frac{1+\cos(t/2)}{2[1-\cos(t/2)]+q^2/4}+\frac{1-\cos(t/2)}{2[1+\cos(t/2)]+q^2/4}\} \tag{III.141}$$

One can convince oneself that $\hat{c}_M^{(n)}(k_0,l)$ displays 2^n distinct simple poles in q^2. Thus, in the parametrisation

$$\hat{c}_M^{(n)}(k_0,l)=\frac{\epsilon_M^2}{q^3}\frac{b_n(q)+c_n(q)\cos(t)}{a_n(q)-\cos(t)} \tag{III.142}$$

$a_n(q)$ must be a polynomial of order 2^n in q^2 whose poles can in principle be read off from the flow equation (III.140). These poles are certain mutually distinct functions of t as one easily sees from the inductive definition (III.140). The flow equation (III.140) for the covariance at resolution M is a superposition of covariances at resolution $2M$ with merely t dependent, positive coefficients $1 \pm \cos(t/2)$ (i.e. they do not depend on q). Since $c_M^{(0)}(k_0, t)$ has its q dependence only in the pole and a single positive coefficient, this feature is preserved for the entire flow. We may therefore display an alternative parametrisation of (III.142) as follows: Let $-[\hat{\lambda}_{MN}^{(n)}(t)]^2$ with $N = -2^{n-1}+1, -2^{n-1}+2, .., 0, 1, .., 2^{n-1}$ denote the poles of $c_M^{(n)}(k_0, l)$ for $n > 0$ with respect to q^2 (from the induction (III.140) it follows that the poles are strictly non-positive) and $\hat{g}_{MN}^{(n)}(t)\epsilon_M^2$ the corresponding, positive coefficient functions. Then, for $n > 0$

$$\hat{c}_M^{(n)}(k_0, l) = \sum_{N=-2^{n-1}+1}^{2^{n-1}} \frac{\hat{g}_{MN}^{(n)}(t)\epsilon_M^2}{q^2 + [\hat{\lambda}_{MN}^{(n)}(t)]^2} \tag{III.143}$$

If we trivially extend $\hat{g}_{MN}^{(n)} \equiv 0$ for $N > 2^{n-1}, N \leq -2^{n-1}$ we may extend the sum over N to infinity

$$\hat{c}_M^{(n)}(k_0, l) = \sum_{N \in \mathbb{Z}} \frac{\hat{g}_{MN}^{(n)}(t)\epsilon_M^2}{q^2 + [\hat{\lambda}_{MN}^{(n)}(t)]^2} \tag{III.144}$$

which now provides a universal parametrisation for the $c_M^{(n)}(k_0, t)$. The flow is now in terms of the poles and their respective coefficient functions. More and more coefficient functions are switched on from zero to a positive function as the flow number n increases. We even know what the fixed point values of this flow are, if we look at (III.132)

$$[\hat{\lambda}_{MN}^*(t)]^2 = (t + 2\pi N)^2, \qquad \hat{g}_{MN}^*(t) = 2\frac{1 - \cos(t)}{(t + 2\pi N)^2} \tag{III.145}$$

The first question is, what null space of the reflection positive inner product for a covariance of the form (III.144) results. It is convenient to introduce the renormalisation invariant lattice Laplacian

$$(\Delta_M f_M)(m) := f_M(m+1) + f_M(m-1) - 2f_M(m) \tag{III.146}$$

on L_M which in Fourier space corresponds to multiplication by $2(\cos(k_M l) - 1) = 2(\cos(t) - 1)$. The functions $\hat{\lambda}_{MN}^{(n)}(t)$, $\hat{g}_{MN}^{(n)}(t)$ can now be considered as the eigenvalues of corresponding operator valued functions of Δ_M which we denote by $\lambda_{MN}^{(n)}, g_{MN}^{(n)}$ respectively. We also set

$$[\omega_{MN}^{(n)}]^2 := \frac{[\lambda_{MN}^{(n)}]^2}{\epsilon_M^2} + p^2 \tag{III.147}$$

Then for the corresponding reflection positive inner product for functions F_M, G_M of positive time support

$$\begin{aligned} & \langle [e^{i\Phi_M[F_M]}]_{\mu_M^{(n)}}, [e^{i\Phi_M[G_M]}]_{\mu_M^{(n)}} \rangle_{\mathcal{H}_M^{(n)}} = \mu_M^{(n)}(e^{i\Phi_M[\theta \cdot G_M - F_M]}) \qquad \text{(III.148)} \\ = \; & \mu_M^{(n)}(e^{i\Phi_M[F_M]})\mu_M^{(n)}(e^{i\Phi_M[G_M]}) \exp(-\sum_N \int ds ds' \int \frac{dk_0}{2\pi} e^{ik_0(s-s')} \langle F_M(s), \frac{g_{MN}^{(n)}}{k_0^2 + (\omega_{MN}^{(n)})^2} G_M(-s') \rangle_{L_M}) \\ = \; & \mu_M^{(n)}(e^{i\Phi_M[F_M]})\mu_M^{(n)}(e^{i\Phi_M[G_M]}) \exp(-\sum_N \int ds ds' \int \frac{dk_0}{2\pi} e^{ik_0(s+s')} \langle F_M(s), \frac{g_{MN}^{(n)}}{k_0^2 + (\omega_{MN}^{(n)})^2} G_M(s') \rangle_{L_M}) \\ = \; & \mu_M^{(n)}(e^{i\Phi_M[F_M]})\mu_M^{(n)}(e^{i\Phi_M[G_M]}) \exp(-\sum_N \int ds \int ds' \langle F_M(s), \frac{g_{MN} \, e^{-(s+s')\omega_{MN}}}{2\omega_{MN}} G(s')_M \rangle_{L_M}) \end{aligned}$$

We now extract representatives of the equivalence classes of the inner product (III.148) corresponding to fields not at a single sharp time zero, but rather a countably infinite set of sharp times. To see how this comes about, we compute, noticing the time support of G and dropping all labels for the sake of the argument

$$\begin{aligned} \int ds \, e^{-s\omega} G(s, m) &= \sum_l \int \frac{dk_0}{2\pi} \int_0^\infty ds \, e^{i(k_0 s + k_M l m)} e^{-s\omega(l)} \hat{G}(k_0, l) \\ = \; & \sum_l \int \frac{dk_0}{2\pi} \frac{1}{\omega(l) - ik_0} e^{ik_M l m} \hat{G}(k_0, l) = -\sum_l e^{ik_M l m} \hat{G}(k_0 = -i\omega(l), l) \end{aligned} \tag{III.149}$$

by the residue theorem. Here we used that $G(s)=0$ for $s<0$ implies that its Fourier transform $\hat{G}(k_0)$ is holomorphic on the lower complex half plane with at most polynomial growth at infinity. Hence the residue theorem applies. It follows that the value of the first expression in (III.149) remains unchanged if we replace $\hat{G}(k_0,l)$ by $\hat{G}'(k_0,l)=h(k_0,l)\;\hat{G}(-i\omega(l),l)$ where h is a fixed function holomorphic in the lower half plane such that $h(-i\omega(l),l)=1$, e.g. $h\equiv 1$.
If we have finitely many frequencies $\omega_N>0$ labelled by $N\in\mathbb{Z}$ then likewise we consider the functions $\hat{G}_N(l):=\hat{G}(-i\omega_N(l),l)$ and can replace $\hat{G}(k_0,l)$ by

$$\hat{G}'(k_0,l)=\sum_N h_N(k_0,l)\;\hat{G}_N(l),\;h_N(-i\omega_{N'}(l),l)=\delta_{N,N'} \tag{III.150}$$

A possible choice is

$$h_N(k_0,l):=\prod_{N'\neq N}\frac{e^{-i\tau k_0}-e^{-\tau\omega_{N'}(l)}}{e^{-\tau\omega_N(l)}-e^{-\tau\omega_{N'}(l)}} \tag{III.151}$$

where $\tau>0$ is any fixed positive real number. (III.151) is well defined because the pole values $\omega_N(l)$ are mutually distinct for different N and equal l. It is holomorphic everywhere and a polynomial in $e^{-ik_0\tau}$ where the order coincides with the number of different frequencies ω_N reduced by one, in our case this number is given by 2^n-1. Thus it becomes a constant at the lower half circle in the complex plane of infinite radius and the residue theorem applies. We conclude that the function $G'(s,m)$ itself, at the n-th renormalisation step, has the form

$$G'(s,l)=\sum_{r=0}^{2^n-1}\delta(s-r\tau)\;g_r(l),\;g_r\in L_M \tag{III.152}$$

i.e. they depend on 2^n sharp points of time rather than a single one, except for $n=0$! It follows that $[e^{i\Phi_M[G_M]}]_{\mu_M^{(n)}}$ can be identified with the representative

$$\frac{\mu_M^{(n)}(e^{i\Phi_M[G_M]})}{\mu_M^{(n)}(e^{i\Phi_M[G'_M]})}\;e^{i\Phi_M[G'_M]} \tag{III.153}$$

or in other words

$$e^{i\Phi_M[G_M]}-\frac{\mu_M^{(n)}(e^{i\Phi_M[G_M]})}{\mu_M^{(n)}(e^{i\Phi_M[G'_M]})}\;e^{i\Phi_M[G'_M]} \tag{III.154}$$

is a null vector with respect to the reflection positive inner product defined by $\mu_M^{(n)}$. The OS Hilbert space $\mathcal{H}_M^{(n)}$ can thus be thought of as the completion of the finite linear span of the $e^{i\Phi_M[G'_M]}$ with G'_M of the form (III.152) and $\Omega_M^{(n)}\equiv 1$.

We compute the corresponding Hamiltonian. This amounts to computing the representative of the equivalence class of $e^{i\Phi_M[T_\beta\cdot F_M]}$ for F_M of the form (III.152). We have

$$(T_\beta\cdot F_M)(s)=F_M(s-\beta)=\sum_r\delta(s-\beta,r\tau)\;f_M^r=\sum_r\delta(s,\beta+r\tau)\;f_M^r \tag{III.155}$$

whence

$$\widehat{T_\beta\cdot F_M}(k_0,l)=\sum_r e^{-ik_0(\beta+r\tau)}\;\hat{f}_M^r(l) \tag{III.156}$$

Thus

$$\begin{aligned}\widehat{T_\beta\cdot F_M}'(k_0,l)&=\sum_N h_{MN}(k_0,l)\;\widehat{T_\beta\cdot F_M}'(-i\omega_{MN}(l),l)=\\&=\sum_N h_{MN}(k_0,l)\;\sum_r e^{-\omega_{MN}(l)(\beta+\tau r)}\;\hat{f}_M^r(l)\end{aligned} \tag{III.157}$$

where h_{MN} is defined as in (III.152) with ω_N replaced by ω_{MN} and we suppressed the renormalisation step label n for notational convenience. If we decompose

$$h_{MN}(k_0,l)=:\sum_r e^{-ir\tau k_0}\;h_{MN}^r(l) \tag{III.158}$$

we obtain

$$\widehat{T_\beta\cdot F_M}'(k_0,l)=\sum_r e^{-ik_0\tau r}\;\sum_{r'}[\sum_N h_{MN}^r(l)\;e^{-\omega_{MN}(l)(\beta+\tau r')}]\;\;\hat{f}_M^r(l) \tag{III.159}$$

Accordingly, the time evolution is described by the matrix

$$A_M^{r,r'}(\beta,l) := \sum_N h_{MN}^r(l)\; e^{-\omega_{MN}(l)(\beta+\tau r')} \tag{III.160}$$

or in position space by the corresponding matrix valued operator where $\omega_{MN}(l)$ is replaced by the corresponding operator. It follows that we can describe the time translation contraction semigroup on the chosen representatives, reintroducing the renormalisation step label, by

$$e^{-\beta H_M^{(n)}} e^{i\Phi_M[F_M]} = \frac{\mu_M^{(n)}(e^{i\Phi_M[F_M]})}{\mu_M^{(n)}(e^{i\Phi_M[A_M^{(n)}(\beta)\cdot F_M]})}\; e^{i\Phi_M[A_M^{(n)}(\beta)\cdot F_M]},\; F_M=\sum_r \delta_{r\tau} f_M^r \tag{III.161}$$

where $A_M^{(n)}(\beta)$ is the purely spatial matrix valued operator whose Fourier transform is displayed in (III.160). It is instructive to verify the semigroup law

$$A_M^{(n)}(\beta_1)\cdot A_M^{(n)}(\beta_2) = A_M^{(n)}(\beta_1+\beta_2) \tag{III.162}$$

which rests on the van der Monde identity for polynomials of degree $d=2^n-1$

$$p(x)=\sum_{r=0}^d a_r\; x^r,\;\; p(x_r)=p_r,\; x_0<x_1<..<x_d \;\;\Rightarrow\;\; p(x)=\sum_{r=0}^d p_r \prod_{r'\neq r}\frac{x-x_{r'}}{x_r-x_{r'}} \tag{III.163}$$

We prove it by applying (III.150) to $h_{MN'}(\omega_{MN}(l)\tau,l)$ in

$$\begin{aligned}&\sum_{r'} A_M^{r,r'}(\beta_1,l)A_M^{r',r''}(\beta_2,l)=\\ &=\sum_{NN'} h_{MN}^r(l)[\sum_{r'} e^{-\omega_{MN}(l)\tau r'} h_{MN'}^{r'}(l)]e^{-\omega_{MN'}(l)\tau r''} e^{-\omega_{MN}(l)\beta_1-\omega_{MN'}(l)\beta_2}=\\ &=\sum_{NN'} h_{MN}^r(l)\delta_{N,N'}e^{-\omega_{MN'}(l)\tau r''} e^{-\omega_{MN}(l)\beta_1-\omega_{MN'}(l)\beta_2}=A_M^{r,r''}(\beta_1+\beta_2)\end{aligned} \tag{III.164}$$

As $n\to\infty$ and for fixed finite M, the Hilbert space can thus no longer be thought of as described by a single sharp time zero field but rather by sharp time fields at an exponentially increasing (with n) number of sharp times. At the fixed point thus, the number of this sharp points of time is actually infinite. How can this be reconciled with the fact that in the continuum the Hilbert space *can* be described by a single field at sharp time zero? The answer lies in the continuum limit $M\to\infty$: If we inspect (III.145) then we see that at fixed $l\in\mathbb{Z}_M$ we obtain for the coupling "constants" $\hat{g}_{MN}(l)\to\delta_{N,0}$ as $M\to\infty$. At the same time $\omega_{MN}(l)$ diverges for all N except $N=0$ and the time contraction for all modes except for $N=0$ "freezes". Thus in the continuum limit, the theory is described by a single dispersion relation and thus the single sharp time zero description that we are used to applies.

The description using fields at more than one sharp time that we have arrived at means that we cannot express the Hamiltonian in terms of a single time zero field and its conjugate momentum. Thus our discussion suggests to introduce instead an infinite number of sharp time zero field species ϕ_{NM} and their conjugate momenta π_{MN}, that is, the non-vanishing commutators are

$$[\pi_{MN}(m),\phi_{MN'}(m')]=i\hbar\delta_{N,N'}\delta_{m,m'},\; m,m'\in\mathbb{Z}_M \tag{III.165}$$

At finite n of course we only have $N\in\{-2^{n-1}+1,..,0,..,2^{n-1}\}$, i.e. we have only $d=2^n$ field species. Accordingly, instead of $L_M=l_2(M)$ we consider $L_M=l_2(M)^d$ as the one particle Hilbert space and the Hamiltonian

$$\begin{aligned}H'_M &:= \frac{1}{2}\sum_{(m,N),(m',N')}[\pi_{MN}(m)D_M((m,N),(m',N'))\pi_{MN'}(m')\\ &\quad+\phi_{MN}(m)E_M((m,N),(m',N'))\phi_{MN'}(m')]\\ &=: \frac{1}{2}[\langle\pi_M,D_M\pi_M\rangle_{L_M}+\langle\phi_M,E_M\phi_M\rangle_{L_M}]\end{aligned} \tag{III.166}$$

for certain operators D_M,E_M on L_M. Then we claim that it is possible to choose D_M,E_M such that the Wiener measure corresponding to (III.166) reproduces the path integral measure. To see this, we drop all labels for simplicity

$$H=\frac{1}{2}[\langle\pi,D\pi\rangle+\langle\phi,E\phi\rangle] \tag{III.167}$$

where D, E are self-adjoint, positive and symmetric on L_M and in general not commuting. We define annihilators and frequency

$$a = \frac{1}{\sqrt{2}}[\langle\kappa, \phi\rangle - i\langle\kappa^{-1}, \pi\rangle],\ H = \langle a^*, \omega' a\rangle \tag{III.168}$$

Note that κ, ω' are operators on L_M. This leads to the identities

$$\kappa^\dagger \omega' \kappa = E,\ (\kappa^{-1})^\dagger \omega' \kappa^{-1} = D \tag{III.169}$$

which are solved by

$$\kappa = \kappa^\dagger > 0,\ \kappa = \sqrt{E^{1/2}\sqrt{E^{-1/2}D^{-1}E^{-1/2}}E^{1/2}},\ \omega' = (\omega')^\dagger > 0,\ \omega' = \kappa D \kappa \tag{III.170}$$

Now a simple computation similar to the one for the continuum that generalises the choice $\kappa = \sqrt{\omega'}$ shows that the Wiener measure corresponding to (III.168) yields

$$\mu(e^{i\Phi[F]}) = e^{-\frac{1}{2}\int\ ds\ \int\ ds' < F(s), \frac{e^{-|s-s'|\omega'}}{2\kappa^2}\ F(s')>} \tag{III.171}$$

We now pick the sharp time zero Weyl elements to be

$$w_M[f'_M] := e^{i\sum_N \phi_{MN}[f'_{MN}]},\ f'_M = \{f'_{MN}\}_N \in L_M^{2^n} \tag{III.172}$$

and also $W_M[F'_M] = \prod_N\ W_{MN}[F'_{MN}],\ W_{MN}[F'_{MN}] = e^{i\Phi_{MN}[F'_{MN}]}$. Then the corresponding Wiener measure gives

$$\mu'_M(W_M[F'_M]) = \exp(-\frac{1}{2}\sum_N \int ds\ \int ds'\ \langle F'_M(s), \frac{e^{-|s-s'|\omega'_M}}{2\kappa_M^2} F'_M(s')\rangle) \tag{III.173}$$

We can use our knowledge from the continuum theory to infer that the Hilbert space corresponding to the reflection positive inner product of μ'_M is labelled by time zero smearing functions $F'_M(s) = \delta(s,0) f'_M$ and that the Hamiltonian is defined by

$$e^{-\beta H'_M} e^{i\phi_M[f'_M]} = \frac{\mu'_M(e^{\Phi_M[\delta_0 f'_M]})}{\mu'_M(e^{\Phi_M[\delta_0 e^{-\beta\omega'_M} f'_M]})}\ e^{i\phi_M[e^{-\beta\omega'_M} f'_M])} \tag{III.174}$$

To match this to (III.161) we perform a trivial relabelling between $r, r', \in \{0, ..., d-1\}$ and $N, N' \in \{-2^{n-1}+1, .., 2^{n-1}\}$ in order to write the matrix elements of A_M in the form $A_M((m, N), (m', N'); \beta)$. Then the semigroup property (III.162) implies that there exists a positive self-adjoint generator ω_M on L_M, such that $A_M(\beta) = e^{-\beta\omega_M}$. Next, for

$$F_M = \sum_{r=0}^{d-1} \delta_{r\tau} f_M^r =: \sum_{N=-2^{n-1}+1}^{2^{n-1}} \delta_{(N+2^{n-1}-1)\tau}\ f_{MN} \tag{III.175}$$

we find a positive matrix B_M on L_M such that

$$\mu_M(e^{i\Phi_M[F_M]}) = e^{-\frac{1}{4}<f_M, B_M f_M>_{L_M}} \tag{III.176}$$

If we now compare (III.161), (III.176) and (III.173), (III.174) we see that we obtain perfect match provided that we pick

$$\omega'_M := \omega_M,\ \ \kappa_M^{-2} := B_M \tag{III.177}$$

Accordingly, the path-integral induced Hamiltonian theory does have an interpretation in terms of sharp zero-time fields, however, at the price of introducing more and more field species at each renormalisation step. These field species are mutually commuting, however, the Hamiltonian couples them to each other according to the matrices D_{RM}, E_{RM} constructed above.

To perform a consistency check on this method, we show that it works for the naively discretised measure, i.e. $n = 0$. In general we have

$$[\hat{\kappa}_{(n)M}^{-2}]^{rr'} = \int \frac{dk_0}{2\pi} e^{ik_0(r-r')} \hat{C}_M^{(n)}(k_0, l) \tag{III.178}$$

with $r, r' \in \mathbb{Z}_{2^n}$ and

$$[\omega_N^{(n)}]^2 = \frac{2}{\epsilon_M} 4^n [1 - \cos(2^{-n}(t + 2\pi N))] + p^2 \tag{III.179}$$

When we use this for (III.140), we obtain

$$[\hat{\kappa}^2_{(0)M}]^{00} = (\int \frac{dk_0}{2\pi}\frac{\epsilon_M^2}{2(1-\cos(t))+p^2+k_0^2})^{-1} = (\frac{2}{\epsilon_M^2}(1-\cos(t))+p^2)^{1/2} \tag{III.180}$$

and as $[A_M^{(n)}]^{00} = e^{-\beta\omega_{M0}^{(0)}}$ we identify immediately $\omega'_M = \omega_{M0}^{(0)}$ and consequently

$$\hat{E} = \frac{2}{\epsilon_M^2}(1-\cos(t))+p^2, \qquad \hat{D} = 1 \tag{III.181}$$

which is consistent with the naive discretisation of the Hamiltonian we started with.
We will also briefly comment on the case $n=1$ as this is the first non-trivial appearance of mixing time fields. First $n=1$ implies that $r=\{0,1\}$. To diagonalise κ_M we note that (III.178) depends on the covariance $\hat{C}_M^{(1)}(k_0,l)$, which is an even function in k_0. We claim that the map

$$U(r,\tilde{r}) = e^{i(r-1)(\tilde{r}-1)\pi} \tag{III.182}$$

diagonalises κ_M, which is easy to check. Consider e.g. the matrix element $\tilde{r}=0, \tilde{r}'=1$ of $(U^\dagger\kappa_M U)(\tilde{r},\tilde{r}')$ then

$$\int dk_0 \sum_{r,r'=0}^{1} e^{i\pi(r-1)}e^{ik_0(r-r')}e^{i\pi\cdot 0}\hat{C}_M^{(1)}(k_0,l) = e^{-i\pi}\int dk_0(e^{i\pi}+1+e^{-ik}-e^{ik})\hat{C}_M^{(1)}(k_0,l) = 0 \tag{III.183}$$

because it is the integral of an even times an odd function. Evaluating in this way:

$$U\hat{\kappa}_M^{-2}U^\dagger = \begin{pmatrix} \int dk_0 2(\sin(k_0)+1)\hat{C}_M^{(1)}(k_0,l) & 0 \\ 0 & \int dk_0 2(\cos(k_0)+1)\hat{C}_M^{(1)}(k_0,l) \end{pmatrix} = \tag{III.184}$$
$$= \begin{pmatrix} 2\int dk_0 \hat{C}_M^{(1)}(k_0,l) & 0 \\ 0 & \int dk_0 2(\cos(k_0)+1)\hat{C}_M^{(1)}(k_0,l) \end{pmatrix} =: \frac{1}{\omega_{M0}(l)\omega_{M1}(l)}\begin{pmatrix} a^2 & 0 \\ 0 & b^2 \end{pmatrix}$$

again because of odd times even.
We can read off directly the h^r_{MN} from

$$h_N(k_0,l) = (-)^N\frac{e^{-i\tau k_0}-e^{-\tau\omega_N(l)}}{e^{-\tau\omega_0(l)}-e^{-\tau\omega_1(l)}} \tag{III.185}$$

Then we will use that $\omega'_M = \partial_\beta A_M(\beta)\mid_{\beta=0}$ and transform this into the basis where $\hat{\kappa}$ is diagonal. After some calculations one finds

$$iU\omega'_M U^\dagger = \begin{pmatrix} e & d \\ \bar{d} & \bar{e} \end{pmatrix} \tag{III.186}$$

and arrives thus at the end result

$$UDU^\dagger = \frac{1}{c}\frac{1}{\omega_{M0}(l)\omega_{M1}(l)}\begin{pmatrix} a^2 e & abd \\ ab\bar{d} & b^2\bar{e} \end{pmatrix}, \qquad UEU^\dagger = \frac{\omega_{M0}(l)\omega_{M1}(l)}{c}\begin{pmatrix} a^{-2}e & a^{-1}b^{-1}d \\ a^{-1}b^{-1}\bar{d} & b^{-2}\bar{e} \end{pmatrix} \tag{III.187}$$

where the quantities ab, c, d, e are given as follows:

$$a := \sqrt{\omega_{M1}(l)^2(1+\cos(t/2))+\omega_{M0}(l)^2(1-\cos(t/2))} \tag{III.188}$$
$$b := \sqrt{\omega_{M1}(l)^2(1+\cos(t/2))(1+\cos(\omega_{M0}(l)))+\omega_{M0}(l)^2(1-\cos(t/2))(1+\cos(\omega_{M1}(l)))} \tag{III.189}$$
$$c := \frac{1}{e^{-\tau\omega_{RM0}(l)}-e^{-\tau\omega_{M1}(l)}} \tag{III.190}$$
$$d := i(e^{\tau\omega_{M0}(l)}+i)(e^{\tau\omega_{M1}(l)}+i)(\omega_{M0}(l)-\omega_{RM1}(l)) \tag{III.191}$$
$$e := -i(e^{\tau\omega_{RM0}(l)}+i)(e^{\tau\omega_{M1}(l)}-i)\omega_{M0}(l)+i(e^{\tau\omega_{M0}(l)}-i)(e^{\tau\omega_{M1}(l)}+i)\omega_{M1}(l) \tag{III.192}$$

Thus, we see that it is possible to write the interaction between the different field species explicitly However, as the interaction becomes quite involved we refer from using this framework in the following and stick to the direct Hamiltonian renormalisation, where the interpretation is more straightforward.

III.C.4 Direct Hamiltonian Renormalisation

We now quote the direct Hamiltonian renormalisation from [129] in terms of the single canonical field species ϕ_M at sharp time zero.

Implementing Isotropy

As already remarked before, implementing isotropy of

$$j^{(n)}_{M\to 2M} e^{i\phi_M[f_M]}\Omega^{(n+1)}_M := e^{i\phi_{2M}[I_{M\to 2M}\cdot f_M]}\Omega^{(n)}_{2M} \tag{III.193}$$

is equivalent to studying the flow of the family of Hilbert space measures

$$\nu^{(n+1)}_M(e^{i\phi_M[f_M]}) := \nu^{(n)}_{2M}(e^{i\phi_{2M}[I_{M\to 2M}\cdot f_M]}) \tag{III.194}$$

Again it is clear that the family stays Gaussian if the original family is. Let $(2\omega^{(0)}_M)^{-1}$ be the covariance of $\nu^{(0)}_M$. We have the basic identity (in the sense of the spectral theorem)

$$\frac{1}{2\omega^{(0)}_M} = \int \frac{dk_0}{2\pi}\frac{1}{k_0^2+(\omega^{(0)}_M)^2} \tag{III.195}$$

which, as in the previous section, can be written in terms of $q^2=(p^2+k_0^2)\epsilon_M^2$ and Δ_M (or $t=k_M l,\ l\in\mathbb{Z}_M$ when Fourier transforming). We now make the self-consistent assumption that the covariance of $\nu^{(n)}_M$ can also be written in the form

$$\frac{1}{2\omega^{(n)}_M} = \int \frac{dk_0}{2\pi}\, c^{(n)}(q,\Delta_M) \tag{III.196}$$

If we compare this to (III.111) then we see that the work has already been done in the previous subsection. Namely, precisely the flow of $\omega^{(n)}_M$ has been computed there, the difference with the current section is that we restrict the smearing fields to the special time dependence $F_M=\delta_0\ f_M$. The integral over k_0 could be explicitly carried out using the residue theorem, in particular for the fixed point covariance in the form displayed in (III.132), which now reads explicitly

$$c^*_M(m,m') = \sum_{l\in\mathbb{Z}_M}\int\frac{dk_0}{2\pi}\hat{c}^*_M(k_0^2+p^2,k_M l), \qquad \hat{c}^*_M(q,t)=\frac{\epsilon_M^2}{q^3}\frac{q\mathrm{ch}(q)-\mathrm{sh}(q)+(\mathrm{sh}(q)-q)\cos(t)}{\mathrm{ch}(q)-\cos(t)} \tag{III.197}$$

However, for what follows we do not need to do this.

Computing the direct Hamiltonian flow

The fixed point sequence is defined by the matrix element equations

$$\begin{aligned}&\langle e^{i\phi_M[f_M]}\Omega^{(n+1)}_M,\ \hat{H}^{(n+1)}_M\ e^{i\phi_M[f'_M]}\Omega^{(n+1)}_M >_{\mathcal{H}^{(n+1)}_M}\\ &:= \langle e^{i\phi_{2M}[I_{M\to 2M}\cdot f_M]}\Omega^{(n)}_{2M},\ \hat{H}^{(n)}_{2M}\ e^{i\phi_{2M}[I_{M\to 2M}\cdot f'_M]}\Omega^{(n)}_{2M}\rangle_{\mathcal{H}^{(n)}_{2M}}\end{aligned} \tag{III.198}$$

Let us define

$$a^{(n)}_M := \frac{1}{\sqrt{2}}[(\omega^{(n)}_M)^{1/2}\phi_M - i(\omega^{(n)}_M)^{-1/2}\pi_M] \tag{III.199}$$

Then

$$\nu^{(n)}_M(e^{i\phi_M[f_M]}) = e^{-\frac{1}{4}\langle f_M,(\omega^{(n)}_M)^{-1}\ f_M\rangle} = \langle\Omega^{(n)}_M,\ e^{i\phi_M[f_M]}\Omega^{(n)}_M\rangle \tag{III.200}$$

is the Fock measure labelled by (III.196) and $\Omega^{(n)}_M$ is the Fock vacuum annihilated by (III.199). Then

$$\begin{aligned}&e^{-i\phi_{2M}[I_{M\to 2M}\cdot f'_M]}\ a^{(n)}_{2M}(m)\ e^{i\phi_{2M}[I_{M\to 2M}\cdot f'_M]}\\ =\ & a^{(n)}_{2M}(m) - i\ [\ \phi_{2M}[I_{M\to 2M}\cdot f'_M]\ ,\ a_M(m)\ ]\\ =\ & a_{2M}(m) + i\sqrt{\frac{\hbar\kappa\epsilon_{2M}^{D/2}}{2}}([\omega^{(n)}_{2M}]^{-1/2}I_{M\to 2M}\cdot f_M)(m)\mathbb{1}_{\mathcal{H}^{(n)}_M}\end{aligned} \tag{III.201}$$

We now prove by induction that

$$\hat{H}^{(n)}_M = \langle a^{(n)}_M, \omega^{(n)}_M \cdot a^{(n)}_M \rangle_{L_M} \tag{III.202}$$

which is consistent with $\hat{H}^{(n)}_M \Omega^{(n)}_M = 0$. By construction, (III.202) holds for $n = 0$ and all M and we assume it to hold up to n and all M. Then

$$\begin{aligned}
& \langle e^{i\phi_{2M}, I_{M\to 2M}\cdot f_M]}\Omega^{(n)}_{2M},\ \hat{H}^{(n)}_{2M}\ e^{i\phi_{2M}[I_{M\to 2M}\cdot f'_M]}\Omega^{(n)}_{2M}\rangle_{\mathcal{H}^{(n)}_{2M}} \\
= \ & \epsilon^D_M \sum_{m,m'} \omega^{(n)}_{2M}(m,m')\ \langle a^{(n)}_{2M}\ e^{i\hat{\phi}_{2M}[I_{M\to 2M}\cdot f_M]}\Omega^{(n)}_{2M},\ a^{(n)}_{2M}\ e^{i\phi_{2M}[I_{M\to 2M}\cdot f'_M]}\Omega^{(n)}_{2M}\rangle_{\mathcal{H}^{(n)}_{2M}} \\
= \ & \frac{\hbar^2\kappa}{2} \sum_{m,m'} \omega^{(n)}_{2M}(m,m')\ \overline{([\omega^{(n)}_{2M}]^{-1/2}\cdot I_{M\to 2M}\cdot f_M)(m)}\ ([\omega^{(n)}_{2M}]^{-1/2}\cdot I_{M\to 2M}\cdot f'_M)(m'),\ \times \\
& \times \langle e^{i\phi_{2M}[I_{M\to 2M}\cdot f_M]}\Omega^{(n)}_{2M},\ e^{i\phi_{2M}[I_{M\to 2M}\cdot f'_M]}\Omega^{(n)}_{2M}\rangle_{\mathcal{H}^{(n)}_{2M}} \\
= \ & \frac{\hbar^2\kappa_\phi}{2}\ \langle I_{M\to 2M}\cdot f_M,\ I_{M\to 2M}\cdot f'_M\rangle_{L_{2M}}\ \langle e^{i\phi_{2M}[I_{M\to 2M}\cdot f_M]}\Omega^{(n)}_{2M},\ e^{i\phi_{2M}[I_{M\to 2M}\cdot f'_M]}\Omega^{(n)}_{2M}\rangle_{\mathcal{H}^{(n)}_{2M}} \\
= \ & \frac{\hbar^2\kappa_\phi}{2}\ \langle f_M,\ f'_M\rangle_{L_M}\ \langle e^{i\hat{\phi}_M[f_M]}\Omega^{(n+1)}_M,\ e^{i\phi_M[f'_M]}\Omega^{(n+1)}_M\rangle_{\mathcal{H}^{(n+1)}_M} \\
=: \ & \langle e^{i\phi_M[f_M]}\Omega^{(n+1)}_M,\ \hat{H}^{(n+1)}_M\ e^{i\phi_M[f'_M]}\Omega^{(n+1)}_M\rangle_{\mathcal{H}^{(n+1)}_M}
\end{aligned} \tag{III.203}$$

where we have made use of isometry of both $I_{M\to 2M}$ and $j^{(n)}_{M\to 2M}$. Thus the matrix elements of $\hat{H}^{(n+1)}_M$ are consistent with (III.202). The fixed point Hamiltonian $\hat{H}^*_M$ is then simply (III.202) with $\omega^{(n)}_R$ replaced by ω^*_M.

We claim that

$$H^*_M = J^\dagger_M H_R J_M \tag{III.204}$$

where H_R is the continuum Hamiltonian and $J_M:\ \mathcal{H}^*_M \to \mathcal{H}^*_R$ the isometric embedding of Fock spaces which is granted to exist due to the equivalence of the fixed point family to an inductive limit Hilbert space family. Indeed, in our case this is simply given by

$$J_M e^{i\phi_M[f_M]}\ \Omega^*_M = e^{i\phi[I_M\cdot f_M]}\ \Omega^*_R \tag{III.205}$$

This follows because the isometry check and $J_{2M}J_{M\to 2M} = J_M$ are equivalent to the corresponding statements for $I_M, I_{M\to 2M}$ and to the statement $(\omega^*_M)^{-1} = I^\dagger_M(\omega^*_R)^{-1}I_M$ for the fixed point covariances of the Hilbert space measures. To prove (III.204) we compute, using the same steps as in (III.203)

$$\begin{aligned}
& \langle e^{i\phi_M[f_{RM}]}\Omega^*_M,\ [J^\dagger_M\hat{H}_R J_M]\ \ e^{i\phi_M[f'_M]}\ \Omega^*_M\rangle_{\mathcal{H}_M} \\
= \ & \langle e^{i\phi_R[I_M\cdot f_M]}\Omega^*_R,\ \hat{H}_R\ \ e^{i\phi_R[I_M\cdot f'_M]}\ \Omega^*_R\rangle_{\mathcal{H}^*_R} \\
= \ & \frac{\hbar^2\kappa_\phi}{2}\ \langle I_M\cdot f_M, I_M\cdot f'_M\rangle_{L_R}\ \langle e^{i\phi[I_M\cdot f_M]}\Omega^*_R,\ \ e^{i\phi[I_M\cdot f'_M]}\ \Omega^*_R\rangle_{\mathcal{H}^*_R} \\
= \ & \frac{\hbar^2\kappa_\phi}{2}\ \langle f_M,\ f'_M\rangle_{L_M}\ \langle e^{i\phi_M[f_M]}\Omega^*_M,\ \ e^{i\phi_M[f'_M]}\ \Omega^*_M\rangle_{\mathcal{H}^*_M} \\
= \ & \langle e^{i\phi_M[f_M]}\Omega^*_M,\ \hat{H}_M\ \ e^{i\phi_M[f'_M]}\ \Omega^*_M\rangle_{\mathcal{H}_M}
\end{aligned} \tag{III.206}$$

as claimed. Thus, not only does there exist a consistent family of Hamiltonian quadratic forms but indeed a fixed point Hamiltonian H^*_R. This Hamiltonian coincides with the one H_R of the continuum because we checked in the previous subsection that the fixed point covariances ω^*_M are obtained from the continuum covariance ω_M by $[\omega^*_M]^{-1} = I^\dagger_M\omega^{-1}_R I_M$.

It is instructive to check that

$$\omega^{-1}_R = \lim_{M\to\infty}(\omega^*_M)^{-1} \tag{III.207}$$

by using the explicit presentation (III.139). To do this note that with $q^2 = (k_0^2 + p^2)\epsilon^2_M$ and $t = k_M l$ we have $\frac{1}{q^3}[q\mathrm{ch}(q) - \mathrm{sh(q)}] \to 1$ as $M \to \infty$ and $\frac{1}{q^3}[\mathrm{sh}(q) - q] \to 1$ as $M \to \infty$ and $\cos(t) \to 1$ and $\frac{\epsilon^2_M}{\mathrm{ch}(q)-\cos(t)} \to \frac{1}{k_0^2+p^2+(k_R l)^2}$. Note also that (III.132) is an instance of the theorem of Mittag-Leffler (see theorem III.E.1) applied to (III.139) that allows to write a meromorphic function as a linear combination of simple pole functions and an entire holomorphic function.

III.D Example: Klein Gordon field II - Properties

The previous section presented an application of the renormalisation procedure. We have seen that a fixed point of the renormalisation flow in both schemes corresponds to cylindrically consistent projections of a continuum theory. However, while it was possible in this example to find the fixed point $(\hat{H}^*_M, \mathcal{H}^*_M, \Omega^*_M)$ by merely studying the fixed point equation thoroughly, this might not be the case anymore in a general situation. Instead, one could consider an initial naive discretisation $(\hat{H}^{(0)}_M, \mathcal{H}^{(0)}_M, \Omega^{(0)}_M)$ and compute the flow of $n \to \infty$. Obviously, the question arises whether this procedure would lead us to the same fixed point, as the one we found by "looking" at the block-spin transformation. For this purpose this section will investigate the properties of the renormalisation procedure as advocated above. Answering among others, how both schemes compare to each other, how the choice of naive discretisation matters and whether the transformation (III.34) leads to the known fixed point and if different choices than $p = 2$ in $I_{M\to pM}$ have impact.
These questions have been studied and answered in [130], hence in the subsections III.D.2-III.D.5 we will copy the calculations therein.

III.D.1 Comparison of the Renormalisation Flow schemes

Upon taking the continuum limit, the path-integral induced Hamiltonian flow agrees with the direct Hamiltonian flow, which is in case of the free scalar field a theory of a single field species. It might be surprising that at coarse resolutions both fixed point theories do look very differently. However, this can be explained as follows:
Given a continuum spacetime measure μ, one can either first consider the cylindrically consistent projections of the mentioned measure, μ_M, and afterwards use the OS reconstruction on it to obtain the OS data $(\mathcal{H}_M, \hat{H}_M, \Omega_M)$ at the same coarse resolution.
Alternatively, starting again from μ we perform first an OS reconstruction to obtain the triple $(\hat{H}, \mathcal{H}, \Omega)$ and afterwards project this onto a coarse resolution, i.e. one constructs an (in general different) triple $(\mathcal{H}'_M, \hat{H}'_M, \Omega'_M)$. If these two quantities do not match, this merely implies that the considered diagram does not close. But although the theories at coarse resolution look different, they still define the same continuum theory.

In case of the free scalar field this is exactly what happens, as we find that the flow of the path-integral induced Hamiltonian renormalisation increases the number of fields species with each step n at finite resolution M, due to the necessity to construct representatives with respect to the null space of the corresponding history space measure. This is exactly, what has been circumnavigated for the direct flow: instead, it stays within a single field species regime for all steps n at every finite resolution M.
But with both defining the same continuum theory, we would be in principle free to choose the scheme, which is technically simpler to execute. Hence, by such practical implications the direct Hamiltonian renormalisation is (at least for the free field) favoured.

Moreover, there is the conceptual advantage of the direct Hamiltonian renormalisation: namely, we would like to obtain the matrix elements of the Hamiltonian at finite resolution. And as we have seen the finite resolution Hamiltonian $\hat{H}^*_M$ of the direct flow is much closer to what we, intuitively, would imagine this object to look like. In contrast to it, the path-integral induced flow has introduced an infinite number of field species at the cylindrically projected level.
Hence, as the first scheme is presenting a more intuitive picture for the interpretation of the objects at finite resolution, we will prefer to work with it in the following.

III.D.2 Convergence and stability of the renormalisation sequence

Let us quickly summarise the results and definitions (III.194),(III.16),(III.102) and (III.108) needed and obtained in the previous section for $\nu^{(n)}_M$, the Hilbert space measure of the 1+1-dimensional Klein-Gordon field of mass p (up to numerical prefactors which are not important for what follows)

$$\begin{aligned}
\nu^{(n)}_M(w_M[f_M]) &= e^{-\frac{1}{2}\langle f_M, c^{(n)}_M f_M\rangle_M} \\
\langle f_M, c^{(n)}_M f_M\rangle_M &:= \epsilon^2_M \sum_{m,m'\in\mathbb{Z}_M} \bar{f}(m)\, c^{(n)}_M(m,m')\, f_M(m') \\
c^{(n)}_M(m,m') : &= c^{(n)}_M(m-m') = \int_{\mathbb{R}} \frac{dk_0}{2\pi} \sum_{l\in\mathbb{Z}_M} e^{ik_M l(m-m')}\, \hat{c}^{(n)}_M(k_0,l) \\
\hat{c}^{(n+1)}_M(k_0,l) &= \frac{1}{2}\Big((1+\cos(lk_M/2)\hat{c}^{(n)}_{2M}(k_0,l) + (1-\cos(lk_M/2)\hat{c}^{(n)}_{2M}(k_0,l+M)\Big) \quad \text{(III.208)}
\end{aligned}$$

where $k_M := \frac{2\pi}{M}$. There we started the recursion with the naive discretisation $(\Delta_M^{(0)} f_M) := \epsilon_M^{-2}[f_M(m+1) + f_M(m-1) - 2f_M(m)]$ of the Laplacian and found that the recursion can be parametrised by three functions $a_n,\ b_n,\ c_n$ of $q_M := \sqrt{k_0^2 + p^2\epsilon_M}$

$$\hat{c}^{(n)}(k_0, l) = \frac{\epsilon_M^2}{q_M^3} \frac{b_n(q_M) + c_n(q_M)\cos(t_M)}{a_n(q_M) - cos(t_M)} \tag{III.209}$$

with $t_M = lk_M$. The flow is then defined in terms of the recursion relations for the parametrising functions

$$\begin{aligned} a_{n+1}(q) &:= 2[a_n(q/2)]^2 - 1, \\ b_{n+1}(q) &:= [2a_n b_n + b_n + c_n + a_n c_n](q/2), \\ c_{n+1}(q) &:= 2[b_n + c_b + a_n c_n](q/2) \end{aligned} \tag{III.210}$$

with the initial values

$$a_0(q) = 1 + q^2/2,\ b_0(q) = q^3/2,\ c_0(q) = 0 \tag{III.211}$$

corresponding to the above chosen naive discretisation of the Hamiltonian. From these the existence of a fixed point was found:

$$a^*(q) = \mathrm{ch}(q),\ b^*(q) = q\mathrm{ch}(q) - \mathrm{sh}(q),\ c^*(q) = \mathrm{sh}(q) - q \tag{III.212}$$

Let us now check whether this fixed point is actually a limit of the recursion or merely an accumulation point. Moreover, the stability of the fixed point with respect to perturbing the initial values was not considered. In what follows we supply the analysis from [130].

Convergence properties

A necessary condition for convergence of the flow is that

$$a_n(q) = 2a_{n-1}(q/2)^2 - 1 \tag{III.213}$$

with starting value $a_0(q) = 1 + \frac{1}{2}q^2$ really runs into its fixpoint

$$\cosh(q) = \sum_n \frac{1}{(2n)!} q^{2n} = 1 + \frac{1}{2}q^2 + \frac{1}{24}q^4 + ... \tag{III.214}$$

We will examine this by computing the flow of the coefficient of each power of q^2 separately. This maps the problem of dealing with recursive functional equations to recursive relations of sequences, see e.g. [215, 216]. One immediately sees that the constant and the quadratic term always remain the same under the flow, i.e. $a_n^{(0)} = 1,\ a_n^{(2)} = \frac{1}{2}$ for all n where $a_n(q) = \sum_{k=0}^{2^{n+1}} a_n^{(k)} q^k$. In fact, it is easy to see that all odd powers of q vanish and that a_n is a polynomial of order 2^n in q^2. For the remaining coefficients we note:

Lemma III.D.1. *Suppose $f, g \in \mathbb{R},\ f \neq 1$. Then for a sequential recursive relation of the form*

$$a_n = f a_{n-1} + g \tag{III.215}$$

we find a solution as:

$$a_n = f^n(a_0 - \frac{g}{1-f}) + \frac{g}{1-f} \tag{III.216}$$

Beweis. It is obviously true for $n = 1$ as $a_1 = fa_0 + \frac{g}{1-f}(1-f) = fa_0 + g$. Assuming thus the claim holds for n it follows

$$a_{n+1} = f\left(f^n(a_0 - \frac{g}{1-f}) + \frac{g}{1-f}\right) + g = f^{n+1}(a_0 - \frac{g}{1-f}) + \frac{g}{1-f} \tag{III.217}$$

□

The lemma can be extended to $f = 1$ using de l'Hospital's theorem.

Lemma III.D.2. *Suppose that $f(n), g(n)$ are sequences with $f(n) \neq 0\ \forall n$. Then a sequential recursive relation of the form:*

$$a_{n+1} = f(n)a_n + g(n) \tag{III.218}$$

is solved by

$$a_n = \left(\prod_{k=0}^{n-1} f(k)\right)\left(a_0 + \sum_{j=0}^{n-1} \frac{g(j)}{\prod_{k=0}^{j} f(k)}\right) \tag{III.219}$$

Beweis. Let $A_n := a_n/(\prod_{k=0}^{n-1} f(k)),\ n \geq 1$ and $A_0 := a_0$. Then by the recursion relation

$$A_{n+1} - A_n = \frac{g(n)}{\prod_{k=0}^{n} f(k)} \tag{III.220}$$

hence

$$A_n - A_0 = \sum_{j=0}^{n-1} A_{j+1} - A_j = \sum_{j=0}^{n-1} \frac{g(j)}{\prod_{k=0}^{j} f(k)} \Rightarrow a(n) = \left(\prod_{k=0}^{n-1} f(k)\right)\left(A_0 + \sum_{j=0}^{n-1} \frac{g(j)}{\prod_{k=0}^{j} f(k)}\right) \tag{III.221}$$

□

It is instructive to verify that Lemma III.D.2 reduces to the previous one when $f(n), g(n)$ do not depend on n.

Since $a_0(q)$ is quadratic and the recursion is quadratic as well, we see that the highest power for $a_n(q)$ is always 2^{n+1}. Now, we apply the Cauchy-product-rule

$$\left(\sum_{k=0}^{\infty} a_k q^k\right)\left(\sum_{k=0}^{\infty} b_k q^k\right) = \sum_{k=0}^{\infty}\left(\sum_{j=0}^{k} a_{k-j} b_j\right) q^k \tag{III.222}$$

to get (using that all the coefficients of all odd powers vanish)

$$a_{n+1}(q) = \sum_{k=0}^{2^{n+2}} a_{n+1}^{(k)} q^k = 2\left(\sum_{k=0}^{2^{n+1}} a_n^{(k)}\left(\frac{q}{2}\right)\right)^2 - 1 = 2\sum_{k=0}^{2^{n+2}}\left(\sum_{j=0}^{k} a_n^{(j)} a_n^{(k-j)}\right) 2^{-k} q^k - 1 \tag{III.223}$$

So as long as $k \geq 4$:

$$a_{n+1}^{(k)} = \sum_{j=0}^{k} a_n^{(j)} a_n^{(k-j)} 2^{-k+1} = 2^{-k+2} a_n^{(k)} + 2^{-k+1} \sum_{j=1}^{k-1} a_n^{(j)} a_n^{(k-j)} \tag{III.224}$$

which is now a linear relation for $a_n^{(k)}$, i.e. we can apply Lemma III.D.2. Now since all $a_l^{(k)} = 0,\ \forall l \leq \lfloor \frac{\ln(k/2)}{\ln 2} \rfloor$ also our starting value is zero and we get:

$$a_m^{(k)} = (2^{-k+2})^m \sum_{t=0}^{m-1} (2^{-k+2})^{-(t+1)}\left(2^{-k+1}\sum_{j=1}^{k-1} a_t^{(j)} a_t^{(k-j)}\right) = \sum_{t=0}^{m-1} \frac{1}{2}(2^{-k+2})^{m-t} \sum_{j=1}^{k-1}\left(a_t^{(j)} a_t^{(k-j)}\right) \tag{III.225}$$

It is easy to compute, e.g.:

$$a_n^{(4)} = \frac{1}{4!}(1 - 2^{-2n}) \tag{III.226}$$

and use this to claim

$$a_n^{(2k)} = \frac{1}{(2k)!}\left(1 + \mathcal{O}(2^{-n})\right), a_n^{(2k+1)} = 0 \tag{III.227}$$

which is the above equation for $k \leq 2$. And assuming it holds for $\forall j \leq k$

$$
\begin{aligned}
a_m^{(2k)} &= (2^{-2k+2})^m \sum_{t=0}^{m-1} (2^{-2k+2})^{-t} \frac{1}{2} \sum_{j=1}^{2k-1} a_t^{(j)} a_t^{(2k-j)} = 2^{2(1-k)m} \sum_{t=0}^{m-1} 2^{2(k-1)t} \frac{1}{2} \sum_{j=1}^{k-1} a_t^{(2j)} a_t^{(2k-2j)} = \\
&= \sum_{t=0}^{m-1} 2^{2(1-k)m-t} \frac{1}{2} \sum_{j=1}^{k-1} \frac{1}{(2j)!(2k-2j)!} \left(1 + \mathcal{O}(2^{-t})\right) \left(1 + \mathcal{O}(2^{-t})\right) \qquad \text{(III.228)}
\end{aligned}
$$

We now expand the function of 2^{-t} appearing in (III.228) as a power series $\sum_i c_i (2^{-t})^i$ with some coefficients $c_i \in \mathbb{R}$, such that the c_i are independent of t and finite. It follows:

$$
\begin{aligned}
a_m^{(2k)} &= \frac{1}{(2k)!} \sum_{j=1}^{k-1} \frac{(2k)!}{(2j)!(2k-2j)!} \frac{1}{2} 2^{2(1-k)m} \left(\sum_{t=0}^{m-1} 2^{2(k-1)t} + \sum_i c_i (2^{-t})^i \right) = \\
&= \frac{1}{(2k)!} \left(\sum_{j=0}^{k} \begin{pmatrix} 2k \\ 2j \end{pmatrix} - 2 \right) 2^{2(1-k)m-1} \left(\frac{1-2^{2(k-1)m}}{1-2^{2(k-1)}} + \sum_i c_i \frac{1-2^{-im}}{1-2^{-i}} \right) \\
&= \frac{1}{(2k)!} \left(\sum_{j=0}^{2k-1} \begin{pmatrix} 2k-1 \\ j \end{pmatrix} - 2 \right) \frac{2^{-m2(k-1)-1}}{2^{2(k-1)}-1} \left(2^{2(k-1)m} - 1 + \sum_i c_i \frac{2^{2(k-1)}-1}{1-2^{-i}} (1-2^{-mi}) \right) \\
&= \frac{1}{(2k)!} (2^{2k-1}-1) \frac{1}{2^{2(k-1)}-1} \left(1 - (2^{-m})^{2(k-1)} + \mathcal{O}(2^{-m}) \right) \\
&= \frac{1}{(2k)!} (1 + \mathcal{O}(2^{-m})) \qquad \text{(III.229)}
\end{aligned}
$$

where we used $\begin{pmatrix} k \\ j \end{pmatrix} := \frac{k!}{j!(k-j)!}$ to obtain line 2 and Pascals rule $\begin{pmatrix} k+1 \\ j \end{pmatrix} = \begin{pmatrix} k \\ j \end{pmatrix} + \begin{pmatrix} k \\ j-1 \end{pmatrix}$ for line 3 and $\sum_{j=0}^{k} \begin{pmatrix} k \\ j \end{pmatrix} = 2^k$ for line 4.

Having shown (III.227), we have also shown that the flow drives the initial value indeed to the fix-point as $n \to \infty$.

Studying the flow of $d_n(q) = b_n(q) + c_n(q)$, however, is considerably more difficult. Although being described by the linear recursion relation $d_{n+1}(q) = 4(1 + a_n(q/2))d_n(q/2)$, not knowing the analytic form of the $a_n(q)$ entering in each step makes it analytically impossible to evaluate exactly whether $d_0 = q^3/2$ flows indeed into $d^*(q) = q(\cosh(q) - 1)$. Instead, we will present the numerical evidence, that it approaches the fixed point rather fast, see figure III.3. We plot the functional dependence as a function of q for different iterations in steps n. At fixed n the deviation from the fixed point is bigger for higher values of q since $a_n(q)$ is a polynomial of degree 2^n. At fixed q the deviation decreases as we increase n.

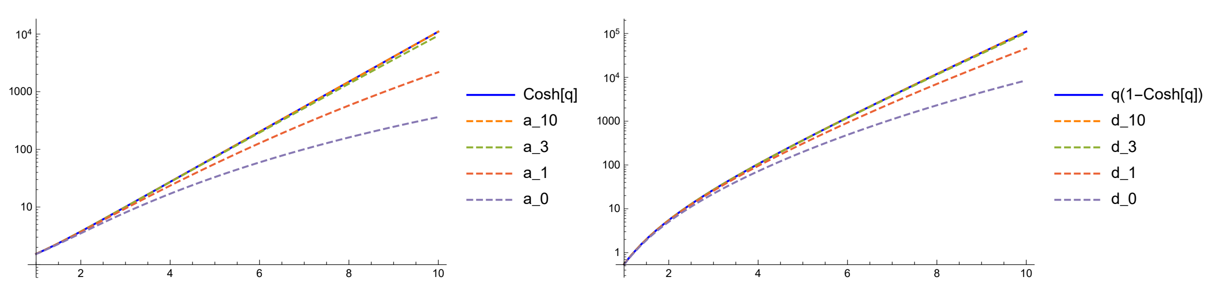

Abbildung III.3: The flow of $a_n(q)$ (left) and $d_n(q)$ (right) for $q \in \{1, 10\}$ in a logarithmic plot. We used dashed lines for the iterations $n = 0, 1, 3, 10$ in different colours and compare this to the corresponding fixed point functions ($a_*(q) = \mathrm{ch}(q)$, $d_*(q) = q(1 - \mathrm{ch}(q))$ as solid blue line. The fixed point is approached from below extremely fast in both cases, such that the blue line is almost indistinguishable from the orange dashed line for $n = 10$ in the depicted interval. The pictures have been taken from [130].

Stability properties with respect to initial conditions

While we have supplied analytical and numerical evidence that starting from the naive lattice Laplacian with only next neighbour contributions the flow indeed converges to the fixed point found, the question arises how stable the fixed point is under changing the initial discretisation of the covariance. In particular, the fact that the flow studied in the previous section was parametrised by three functions only, rests on the form of the initial discretisation. If we also consider initial discretisations that involve next to next neighbour contributions, then a parametrisation by three functions is no longer sufficient as we will see. The most general, translation invariant, symmetric form of the lattice Laplacian on a one dimensional lattice consisting of M points is given by (note the periodicity of the function)

$$(\Delta_M f_M)(m) = \frac{1}{\epsilon_M^2} \sum_{k=0}^{\lfloor M/2 \rfloor} \Delta_M(k)[f_M(m+k) + f_M(m-k)] \tag{III.230}$$

where the M coefficients $\Delta_M(k)$ are such that for $f_M = E_M f,\ f \in C^\infty([0,R))$ the Taylor expansion up to second order in ϵ_M yields $f''(m\epsilon_M)$. We call this a *physically allowed discretisation*. This gives the two constraints

$$\sum_{k=0}^{\lfloor M/2 \rfloor} \Delta_M(k) = 0,\ \sum_{k=1}^{\lfloor M/2 \rfloor} \Delta_M(k) k^2 = 1 \tag{III.231}$$

leaving $M-2$ free parameters for the allowed discretisations. As an example, consider the next to next neighbour case, i.e. $\Delta_M(k) = 0, k > 2$ leaving one free parameter γ

$$(\Delta_M^\gamma f_M)(m) = \frac{\epsilon_M^{-2}}{1+4\gamma}([f(m+1) + f(m-1) - 2f(m)] + \gamma[f(m+2) + f(m-2) - 2f(m)]) \tag{III.232}$$

The case $\gamma = 0$ reproduces the naive next neighbour Laplacian, thus $\gamma \in \mathbb{R}$ labels its next to next neighbour type of perturbation.

As an example, we consider a choice for γ within the next to next neighbour discretisation class which makes $\Delta_M E_M f$ agree with $E_M \Delta f$ up to order ϵ_M^4. The power expansion of $f(x \pm \epsilon),\ \epsilon \equiv \epsilon_M$ and $f(x \pm 2\epsilon)$ results in the following linear system:

$$\begin{pmatrix} f(x+\epsilon) - f(x) \\ f(x+2\epsilon) - f(x) \\ f(x-\epsilon) - f(x) \\ f(x-2\epsilon) - f(x) \end{pmatrix} = \begin{pmatrix} 1 & 1/2 & 1/6 & 1/24 \\ 2 & 2 & 4/3 & 2/3 \\ -1 & 1/2 & -1/6 & 1/24 \\ -2 & 2 & -4/3 & 2/3 \end{pmatrix} \begin{pmatrix} \epsilon f'(x) \\ \epsilon^2 f''(x) \\ \epsilon^3 f^{(3)}(x) \\ \epsilon^4 f^{(4)}(x) \end{pmatrix} \tag{III.233}$$

If one inverts the appearing matrix, one can read of the contributions for f'' which are

$$(\Delta f)(x) = f''(x) = \frac{1}{12\epsilon^2}\left(-f(x+2\epsilon) - f(x-2\epsilon) + 16f(x+\epsilon) + 16f(x-\epsilon) - 30f(x)\right) \tag{III.234}$$

This corresponds to the choice $\gamma = -\frac{1}{16}$.

Its eigenvalues in the Fourier basis are (using $\cos(2x) = 2\cos(x)^2 - 1$)

$$\begin{aligned}(\Delta e^{ikn\cdot})(x) &= \frac{e^{iknx}}{12\epsilon^2}\left(-e^{ikn2} - e^{-ikn2} + 16(e^{ikn} + e^{-ikn}) - 30\right) = \\ &= -\frac{e^{iknx}}{6\epsilon^2}\left(\cos(2kn) - 16\cos(kn) + 15\right) = \\ &= -\frac{1}{3\epsilon^2} e^{iknx}\left((\cos(kn) - 4)^2 - 9\right) =: \hat{\Delta}(n) e^{iknx}\end{aligned} \tag{III.235}$$

Accordingly, the initial covariance is now, described by (recall $q^2 = (k_0^2 + p^2)\epsilon_M^2$, the appearing constants are irrelevant for what follows)

$$\begin{aligned}\hat{C}_M^{(0)}(k_0, l) &= R^{-1}\frac{\hbar\kappa_\phi}{2}\frac{3\epsilon_M^2}{(\cos(k_M l) - 4)^2 - 9 + 3\epsilon_M^2(p^2 + k_0^2)} \\ &= R^{-1}\frac{\hbar\kappa}{2}\frac{3\epsilon_M^2}{\cos(k_M l)^2 - 8\cos(k_M l) + 7 + 3q^2}\end{aligned} \tag{III.236}$$

Let $C_M^{(n)} = \hbar\kappa_\phi c_M^{(n)}/R$. The renormalisation flow (for $D=1$) is given by

$$\hat{c}_M^{(n+1)}(l,k_0) = \frac{1}{2}\Big([1+\cos(k_{2M}l)]\hat{c}_{2M}^{(n)}(l,k_0) + [1-\cos(k_{2M}l)]\hat{c}_{2M}^{(n)}(l+M,k_0)\Big) \tag{III.237}$$

We claim that this transformation leaves invariant the following functional form parametrised by six functions $a_n, ..., f_n$ $(t = k_M l)$

$$\hat{C}_M^{(n)}(t) = \frac{\epsilon_M^2}{q^3}\frac{f_n(q)\cos(t)^2 + e_n(q)cos(t) + d_n(q)}{c_n(q)\cos(t)^2 - b_n(q)\cos(t) + a_n(q)} \tag{III.238}$$

The initial data can be read off from (III.236)

$$a_0 = 7+3q^2, \;\; b_0 = 8, \;\; d_0 = 3q^3, \;\; e_0 = 0, \;\; f_0 = 0, \;\; c_0 = 1 \tag{III.239}$$

After one renormalisation step, the denominator becomes the product

$$\begin{aligned}
&2[c_n\cos(t)^2 - b_n\cos(t) + a_n][c_n\cos(t)^2 + b_n\cos(t) + a_n] = \\
&\quad = 2\left(c_n^2\cos(t)^4 + a_n^2 + 2a_nc_n\cos(t)^2 - b_n^2\cos(t)^2\right) = \\
&\quad = 2\left(c_n^2/4 + c_n^2/4\cos(2t)^2 + c_n^2/2\cos(2t) + a_nc_N\cos(2t) + a_nc_n - b_n^2\cos(2t) - b_n^2 + a_n^2\right) = \\
&\quad = [c_n^2/2]\cos(2t)^2 - [b_n^2 - c_n^2 - 2a_nc_n]\cos(2t) + [c_n^2/2 + 2a_nc_n - b_n^2 + 2a_n^2]
\end{aligned} \tag{III.240}$$

Remembering that under the renormalisation we have $t \mapsto t/2$, $q \mapsto q/2$, we can read off the recursion relations

$$c_{n+1}(2q) := c_n(q)^2/2 \tag{III.241}$$
$$b_{n+1}(2q) := b_n^2(q) - c_n(q)\left(c_n(q) + 2a_n(q)\right) \tag{III.242}$$
$$a_{n+1}(2q) := c_n(q)\left(c_n(q)/2 + 2a_n(q)\right) - b_n^2(q) + 2a_n^2(q) \tag{III.243}$$

For c_n we can immediately see that $n \to \infty$ flows into the fixed point $c_*(q) = 0$. Then the fixed point condition for (III.242) becomes $b_*(2q) = b_*(q)^2$. This functional equation has the one parameter set of solutions $\alpha \mapsto b_*(q) = e^{\alpha q}$. Our initial condition (III.239) started with a function $b_0(q)$ that was even in q and (III.242) does not change this behaviour. Thus the only choice is: $\alpha = 0, b_*(q) = 1$.
Consequently, we find the fixed point condition for (III.243)

$$a_*(2q) = 2a_*(q)^2 - 1 \tag{III.244}$$

already familiar from the next neighbour discretisation class and which is solved by the functions $\cos$ and $\cosh$. Looking now at the numerator from (III.237)

$$\begin{aligned}
&2(1+\cos(t/2))\left[f_n\cos(t/2)^2 + e_n\cos(t/2) + d_n\right]\left[c_n\cos(t/2)^2 + b_n\cos(t/2) + a_n\right] + \\
&+ 2(1-\cos(t/2))\left[f_n\cos(t/2)^2 - e_n\cos(t/2) + d_n\right]\left[c_n\cos(t/2)^2 - b_n\cos(t/2) + a_n\right] = \\
&= [f_nc_n + f_nb_n + e_nc_n]\cos(2t)^2 + \\
&\quad + 2[f_nc_n + f_nb_n + e_nc_n + f_na_n - e_nb_n + d_nc_n + e_na_n + b_nd_n]\cos(2t) + \\
&\quad + 2[f_nc_n/2 + f_nb_n/2 + e_nc_n/2 + f_na_n + e_nb_n + d_nc_n + e_na_n + b_nd_n + 2a_nd_n]
\end{aligned} \tag{III.245}$$

Hence, the remaining recursion relations are

$$f_{n+1}(2q) := \left(f_nc_n + f_nb_n + e_nc_n\right)(q) \tag{III.246}$$
$$e_{n+1}(2q) := 2\left((f_n + e_n + d_n)c_n + (a_n + b_n)f_n + e_nb_n + d_nb_n + e_na_n\right)(q) \tag{III.247}$$
$$d_{n+1}(2q) := 2\left(\frac{1}{2}(2d_n + f_n + e_n)c_n + \frac{1}{2}(2a_n + b_n)f_n + 2a_nd_n + e_nb_n + b_nd_n + e_na_n\right)(q) \tag{III.248}$$

Plugging in the already known results (i.e. $c_* = 0$, $b_* = 1$ and $a_* \in \{\cosh(q), \cos(q)\}$) we find that the fixed point of f_n must obey

$$f_*(2q) = f_*(q) \tag{III.249}$$

The only scale invariant function in one variable is a constant, i.e $f_* = K$. To see which value of K is picked by the initial conditions it is sufficient to compute the flow at $q = 0$. We notice that $d_0(0) = e_0(0) = f_0(0) = 0$

and that (III.246)-(III.248) is a homogeneous system of equations of first order as far as the functions d_n, e_n, f_n are concerned. This means, by induction, that the values of d_n, e_n, f_n at $q = 0$ remain zero for the entire flow. It follows that: $K = 0$. The remaining fixed point conditions reduce then to those for the next neighbour class discretisation, i.e. compare to (III.210)

$$2e_*(2q) = 2(2 + a_*)e_* + 2d_*, \qquad d_*(2q) = (2a_* + 1)d_* + (a_* + 1)(2e_*) \tag{III.250}$$

It follows that both the (unique) choice from the next neighbour class and the above choice from the next to next neighbour class have the same unique fixed point.

Concerning the convergence of the system towards the fixed point, the situation is more involved than for the next neighbour class. While by similar methods $c_n(q)$ is explicitly computable as

$$c_n(q) = 2^{-\sum_{k=0}^{n} 2^k} = 2^{1-2^{(1+n)}} \tag{III.251}$$

it turns out that if we start with the initial values from (III.239) one finds that the flow of a_n, b_n, d_n, e_n, f_n for each coefficient of the respective power series diverges. Consider for instance $a_n(0)$. As $c_n(q)$ approaches zero exponentially fast this means the for higher iterations we approach for $a_n(0)$ the recursive equation $a_{n+1}(0) = 2a_n(0)^2 - 1$. Let $\delta_n = a_n(0) - 1$ then $\delta_{n+1} = 2\delta_n(2 + \delta_n)$. This means that the error δ_n grows exponentially, i.e. $a_n(0)$ appears to be a *relevant coupling* in the terminology of statistical physics. For starting values $|a_0(0)| > 1$ the sequence diverges. For starting values $|a_0(0)| < 1$ the sequence displays chaotic behaviour and does not converge to the fixed point but there may be a subsequence that does. Our chosen discretisation picks $a_0(0) = 7$ so certainly $a_n(0)$ by itself does not converge.

Note however, that the convergence of the coefficient function sequences $a_n, .., f_n$ is only sufficient for the convergence of the covariance. Indeed, since the covariance is a homogeneous rational function of those six functions, that is, a fraction with both numerator and denominator linear in those functions, after each renormalisation step a common rescaling of those functions by any (non vanishing) other function such as a (non vanishing) constant leaves the covariance unaffected. It turns out that a common rescaling by $b_n(0)$ after each renormalisation step leads to modified sequences

$$a'_n(q) := \frac{a_n(q)}{b_n(0)}, \; .. \; f'_n(q) := \frac{f_n(q)}{b_n(0)} \tag{III.252}$$

which now converge as the numerical evidence suggests. Even more, the convergence takes place independently of the value of γ except for $\gamma = \gamma_0 = -\frac{1}{4}$ which plays a special role as the discretisation of the Laplacian blows up here.

We plot both the individual functions at $\gamma = -1/16$ and the total covariance at two values of γ smaller and bigger than γ_0. The convergence of the covariance is faster for $\gamma > \gamma_0$ since for $\gamma < \gamma_0$ the denominator can become small. However, the position of those minima moves to infinity as the flow proceeds. It is clear from this section how one would repeat the analysis, e.g., for the next to next to next neighbour class where one would have a two-parameter freedom. We leave this for future work.

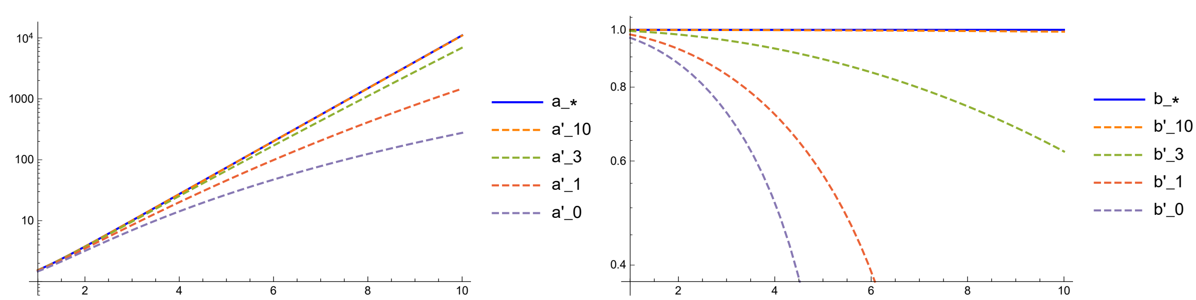

Abbildung III.4: The flow of the rescaled $a'_n(q)$ (left) and $b'_n(q)$ (right) for $q \in \{1, 10\}$ in a logarithmic plot. We used dashed lines for the iterations $n = 0, 1, 3, 7, 10$ in different colours and compare to this the corresponding fixed point functions ($a_*(q) = \mathrm{ch}(q)$, $b_*(q) = 1$) as a solid blue line. The fixed point is approached from below extremely fast in both cases, such that the blue line is almost indistinguishable from the orange dashed line for $n = 10$ in the depicted interval. Note that we do not display $c'_n(q)$ which approaches zero exponentially fast. The pictures have been taken from [130].

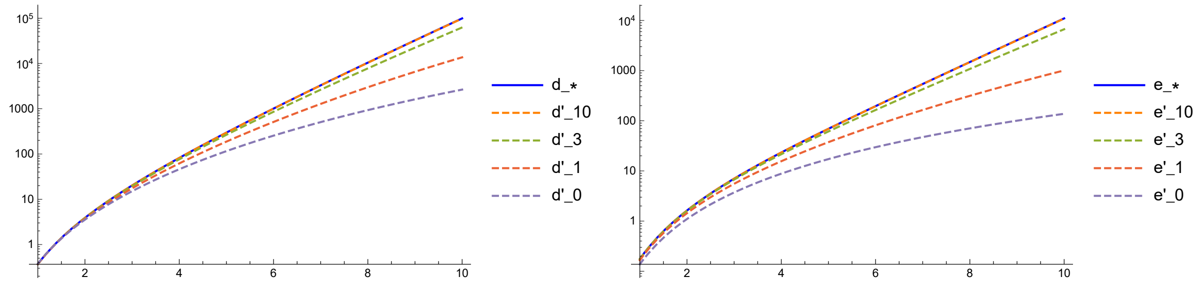

Abbildung III.5: The flow of the rescaled $d'_n(q)$ (left) and $e'_n(q)$ (right) for $q \in \{1, 10\}$ in a logarithmic plot. We use dashed lines for the iterations $n = 0, 1, 3, 7, 10$ in different colours and compare to this the corresponding fixed point functions $(d_*(q) = q\mathrm{ch}(q) - \mathrm{sh}(q)$, $e_*(q) = \mathrm{sh}(q) - q)$ as a solid blue line. The fixed point is approached from below extremely fast in both cases, such that the blue line is almost indistinguishable from the orange dashed line for $n = 10$ in the depicted interval. Note that we do not display $f'_n(q)$ which approaches zero exponentially fast. The pictures have been taken from [130].

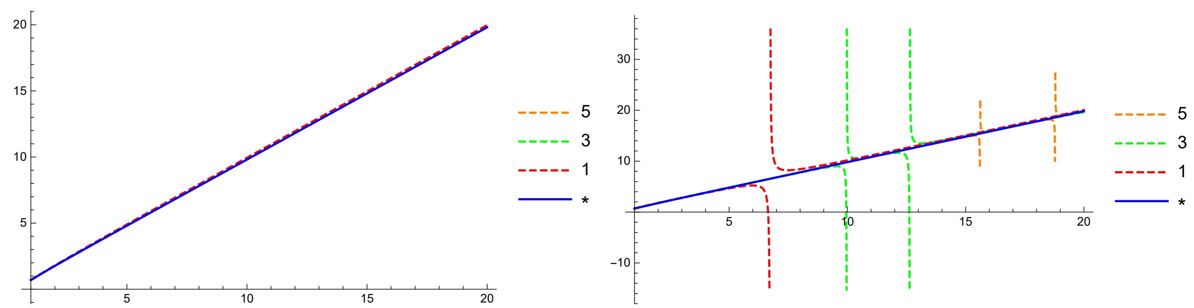

Abbildung III.6: The flow of the total covariance $\hat{C}^{(n)}(q, t = 2\pi/10)$ as function of $q \in [1, 20)$ for various iterations $n = 1, 3, 5$ of the RG map. On the left the naive discretisation to start the flow with was $\gamma = 1/3 > \gamma_0$ and on the right it was $\gamma = -1/3 < \gamma_0$. On the left, we find that the fixed point is approached very rapidly and on the right we see that, although the number of poles grows, they get shifted towards infinity for increasing n. The pictures have been taken from [130].

III.D.3 Universality Properties

The flow - and correspondingly the final fix-point - of the measure family imposes the cylindrical consistency condition on the coarse graining maps, hence only a certain subset of all possible coarse graining maps $I_{M\to 2M}$ can be considered. However, it transpired in [130] that the *block-spin*-map considered so far is not unique. In this subsection we quote the investigations on other suggestions from there, e.g. the *deleting*-map, which is also cylindrically consistent. Moreover, in this subsection we study the latter in the context of direct Hamiltonian renormalisation. In the following subsection, III.D.4, we will make the comparison to the literature and compute the fixed points of deleting and block-spin map in the path integral context in the formalism which is used in the standard literature.

To review the notation, we consider the discretised Weyl element smeared with the test function f_M:

$$w_M[f_M] = \exp\left(i \sum_{m\in\mathbb{Z}_M} \phi_M(m) f_M(m)\right) \tag{III.253}$$

which allows us to define the generating functional of the Hilbert space measure ν_M as:

$$\nu_M(w_M[f_M]) = \int d\nu_M(\phi_M) e^{i\phi_M[F_M]} \tag{III.254}$$

where in practice $d\nu_M(\phi^M)$ is a suitable weight function times M-copies of the Lebesque measure in $\phi_M(m)$.

The map $(I_{M\to 2M} f_M)(m) = f_M(\lfloor m/2 \rfloor)$, $m \in \mathbb{Z}_{2M}$ which we had considered so far allows us to rewrite the *cylindrical consistency condition*

$$\nu_M(w_M[f_M]) = \nu_{2^n M}(w_{2^n M}[I_{M\to 2^n M} f_M]) \tag{III.255}$$

e.g. for $n=1$ as

$$\int d\nu_M(\phi_M)e^{i\phi_M[f_M]} = \int d\nu_{2M}(\phi_{2M})e^{i\phi_{2M}[I_{M\to 2M}f_M]} = \\ = \int d\nu_{2M}(\phi_{2M})e^{i\sum_{m\in\mathbb{Z}_{2M}} f_M(\lfloor m/2\rfloor)\phi_{2M}(m)} \\ = \int d\mu_{2M}(\phi_{2M})e^{i\sum_{m'\in\mathbb{Z}_M} f_M(m')\left(\phi_{2M}(2m')+\phi_{2M}(2m'+1)\right)} \tag{III.256}$$

which shows that $I_{M\to 2M}$ indeed represents a block-spin-transformation in the usual sense.

However, the flow of measures certainly depends on the chosen block-spin-transformation and thus also the fixed points could depend on it. The degree of independence of the choice of such a map $\tilde{I}_{M\to 2M}$ is loosely referred to as *universality*. For example, the *deleting map* is defined by

$$\left(I^{Del}_{M\to 2M}f_M\right)(m) = \begin{cases} 2^\alpha f_M(m/2) & \text{if } m\in 2\mathbb{Z}_M \\ 0 & \text{else} \end{cases} \tag{III.257}$$

As one can check, this map passes *the cylindrical consistency condition* from Lemma III.A.1 for any $\alpha\in\mathbb{R}$

$$I^{Del}_{2^nM\to 2^{n+n'}M}\circ I^{Del}_{M\to 2^nM} = I^{Del}_{M\to 2^{n+n'}M} \tag{III.258}$$

However, the only way to guarantee that this map is isometric is $\alpha = D/2$ because

$$\langle f_M, f'_M\rangle_M = \epsilon_M^D\sum_{m\in\mathbb{Z}_M^D}\bar{f}_M(m)f'_M(m) = \langle I^{Del}_{M\to 2M}f_M, I^{Del}_{M\to 2M}f'_M\rangle_M = \\ = \epsilon_{2M}^D\sum_{m\in 2\mathbb{Z}^D_{2M}} 2^{2\alpha}f_M(m/2)f'_M(m/2) = 2^{2\alpha-D}\epsilon_M^D\sum_{m\in\mathbb{Z}_M^D}f_M(m)f'_M(m) \tag{III.259}$$

We refrain from constructing explicit evaluation and injection maps, since they are irrelevant for determining the fixed point as well as taking the inductive limit. We will study it below and compare with the transformation used in the previous section.

The set of coarse graining transformations satisfying cylindrical consistency is infinite (e.g. one could use $I_{M\to pM}$ instead of $I_{M\to 2M}$ where p is any prime number). Yet, these are indeed non-trivial conditions, and not all renormalisation-flows studied in the literature fulfil these conditions. E.g. in the literature it is standard to consider the *approximate blocking kernel* (see e.g. [106, 112–114] and reference therein)

$$e^{i\phi_{2M}[I^\kappa_{M\to 2M}F_M]} := \int d\tilde{\phi}_M e^{-2\kappa[\sum_{m\in\mathbb{Z}_M}(\tilde{\phi}_M(m)-\frac{1}{2}\sum_{m'\in\mathbb{Z}_{2M},\lfloor m'/2\rfloor=m}\phi_{2M}(m'))]^2} e^{i\tilde{\phi}_M[f_M]} \tag{III.260}$$

For $\kappa\to\infty$ the exponential tends to the δ-Dirac-distribution and reproduces the renormalisation map, $I_{M\to 2M} = \lim_{\kappa\to\infty} I^\kappa_{M\to 2M}$ which as we know satisfies the cylindrical consistency condition.

We review the renormalisation flow based on the approximate blocking transformation in the next section. To see that our renormalisation flow $n\mapsto\nu_M^{(n)}$ is consistent with the flow used in the literature (which we will be defined in (III.272)) in terms of action functionals we write $d\nu_M^{(n+1)}(\phi_M) = d^M\phi_M e^{-\beta S_M^{(n+1)}(\phi_M)}$ with $S_M^{(n+1)}(\phi_M)$ being a function of ϕ_M ("action functional"), then:

$$\nu_M^{(n+1)}(w_M[f_M]) = \int d^M\phi_M\left(e^{-\beta S_M^{(n+1)}(\phi_M)}\right)e^{i\phi_M[f_M]} \stackrel{(III.254)}{=} \int d\nu_{2M}^{(n)}(\phi_{2M})e^{i\phi_{2M}[I^\kappa_{M\to 2M}f_M]} \\ \stackrel{(III.260)}{=} \int d^M\tilde{\phi}_M\left(\int d\nu^{(n)}_{2M}(\phi_{2M})e^{-2\kappa[\sum_{m\in\mathbb{Z}}(\tilde{\phi}_M(m)-\frac{1}{2}\sum_{m'\in\mathbb{Z}_{2M},\lfloor m'/2\rfloor=m}\phi_{2M}(m'))]^2}\right)e^{i\tilde{\phi}_M[f_M]} \tag{III.261}$$

Cylindrical Inconsistency of the Approximate Blocking Kernel

We check whether (III.258) holds for any $\infty>\kappa>0$. If true, then a necessary implication would be that

$$e^{i\phi_{4M}[I^\kappa_{M\to 4M}f_M]} \stackrel{?}{=} e^{i\phi_{4M}[I^\kappa_{2M\to 4M}\circ I^\kappa_{M\to 2M}f_M]} \tag{III.262}$$

which reads explicitly

$$\int d^{2M}\tilde{\phi}_{2M} e^{-2\kappa\sum_{m\in\mathbb{Z}_{2M}}[\tilde{\phi}_{2M}(m)-\frac{1}{2}\sum_{m'\in\mathbb{Z}_{4M},\lfloor m'/2\rfloor=m}\phi_{4M}(m')]^2}\times$$
$$\times\int d^M\phi'_M e^{-2\kappa\sum_{n\in\mathbb{Z}_M}[\phi'_M(m)-\frac{1}{2}\sum_{n\in\mathbb{Z}_{2M},\lfloor n'/2\rfloor=n}\tilde{\phi}_{2M}(n')]^2}$$
$$\stackrel{?}{=}\int d^M\phi'_M e^{-2\kappa\sum_{m\in\mathbb{Z}_M}[\phi'_M-\frac{1}{4}\sum_{m'\in\mathbb{Z}_{4M},\lfloor m'/4\rfloor=m}\phi_{4M}(m')]^2}e^{i\phi'_M[f_M]} \tag{III.263}$$

We evaluate the Gaussians on the left hand side:

$$\int d^{2M}\tilde{\phi}_{2M}\exp(-2\kappa\sum_{m\in\mathbb{Z}_{2M}}\tilde{\phi}_{2M}(m)^2-\kappa/2\sum_{m\in\mathbb{Z}_{2M}}\tilde{\phi}_{2M}(m)^2)\times$$
$$\times\exp(-\kappa/2\sum_{n\in\mathbb{Z}_M}\tilde{\phi}_{2M}(2n)\tilde{\phi}_{2M}(2n+1))\exp(-2\kappa\sum_{m\in\mathbb{Z}_{2M}}\tilde{\phi}_{2M}(m)A(m)) \tag{III.264}$$

where we defined $A(m):=\sum_{m'\in\mathbb{Z}_{4M},\lfloor m'/2\rfloor=m}\phi_{4M}(m')+\phi'_M(\lfloor m/2\rfloor)$.
We perform the integrals over $\tilde{\phi}_{2M}(2n+1),\ n\in\mathbb{Z}_M$ first and then perform the remaining integral over $\tilde{\phi}_{2M}(2n),\ n\in\mathbb{Z}_M$, denoted by $d^M\tilde{\phi}_{2M}$, resulting in

$$\int d^M\tilde{\phi}_{2M}\sqrt{\frac{2\pi}{5\kappa}}^M e^{\kappa/10\sum_{n\in\mathbb{Z}_M}(\frac{1}{2}\tilde{\phi}_{2M}(2n)+2A(2n+1))^2}e^{-5\kappa/2\sum_{n\in\mathbb{Z}_M}\tilde{\phi}_{2M}(2n)^2}e^{-2\kappa\sum_{n\in\mathbb{Z}_M}\tilde{\phi}_{2M}(2n)A(2n)}=$$
$$=\sqrt{\frac{2\pi}{5\kappa}}^M e^{2\kappa/5\sum_{n\in\mathbb{Z}_M}A(2n+1)^2}\int d^M\tilde{\phi}_{2M}e^{\sum_{n\in\mathbb{Z}_M}\tilde{\phi}_{2M}(2n)^2(1/40-5/2)\kappa-\sum_{n\in\mathbb{Z}_M}\tilde{\phi}_{2M}(2n)(2\kappa A(2n)-\kappa/5A(2n+1))}$$
$$=\sqrt{\frac{2\pi}{5\kappa}}^M\sqrt{\frac{40\pi}{99\kappa}}^M e^{\frac{2\kappa}{5}\sum_{n\in\mathbb{Z}_M}A(2n+1)^2}e^{\frac{10}{99}\kappa\sum_{n\in\mathbb{Z}_M}(2A(2n)-1/5A(2n+1))^2} \tag{III.265}$$

It is transparent, that e.g. the coefficients of the $\phi'_M(n)^2,\ n\in\mathbb{Z}_M$ appearing in the exponent of the last line above do not sum up to -2κ. It follows that $I^\kappa_{M\to 2M}$ does not fulfil the cylindrical consistency condition for any finite κ and we exclude it from the list of acceptable blocking kernels.

Continuum theory for different blocking-kernels

Both the deleting kernel and the kernel we used so far are cylindrically consistent. How do their flows compare to each other?

To answer this question, we investigate the path-integral induced flow of the covariance

$$C_M^{Del,(n+1)}=(1_{L_T}\otimes I^{Del}_{M\to 2M})^\dagger C_{2M}^{Del,(n)}(1_{L_T}\otimes I^{Del}_{M\to 2M}) \tag{III.266}$$

which can be computed using the same methods as before:

$$\langle F_M,C_M^{Del,(n+1)}F_M\rangle_M=$$
$$=\epsilon_{2M}^{2D}\sum_{m_1,m_2\in\mathbb{Z}^D_{2M}}\int ds\int ds'\times$$
$$\times(1_{L_T}\otimes I^{Del}_{M\to 2M}F_M)(s,m_1)(1_{L_T}\otimes I^{Del}_{M\to 2M}F_M)(s',m_2)C_{2M}^{Del,(n)}((s,m_1),(s',m_2))=$$
$$=\frac{2^{2\alpha}}{2^{2D}}\epsilon_M^{2D}\int ds\int ds'\sum_{m_1,m_2\in\mathbb{Z}^D_M}F_M(s,m_1)F_M(s',m_2)C_{2M}^{Del,(n)}(s,m_1),(s',m_2)) \tag{III.267}$$

Which tells us that the flow of the covariance is given by

$$C_M^{Del,(n+1)}((s,m_1),(s',m_2))=2^{2(\alpha-D)}C_{2M}^{Del,(n)}((s,m_1),(s',m_2)) \tag{III.268}$$

and consequently, also for their discrete Fourier transforms. We find this to drive the $D=1$ starting covariance

$$\hat{C}_M^{(0)}(k_0,l)=R^{-1}\frac{\hbar\kappa}{2}\frac{1}{\epsilon_M^{-2}(1-\cos(k_Ml))+k_0^2+p^2} \tag{III.269}$$

to zero or infinity unless $\alpha = D$. This demonstrates two things: First, the isometry of the coarse graining map is not a necessary condition in order to define a suitable flow. On the other hand, by far not every map defines a meaningful flow.

Picking $\alpha = D$ we compare the continuum limits $M \to \infty$ of both fixed point covariances computed by the block spin and deleting kernel respectively

$$\lim_{M\to\infty} C^*_M(k_0,l) = \frac{\hbar\kappa}{4R}\frac{1}{p^2+k_0^2+(2\pi l)^2} = \lim_{M\to\infty} C_M^{Del,*}(k_0,l) \tag{III.270}$$

Thus the two continuum theories they define are identical when $\alpha = D$. Note that, trivially, the cylindrical projections of the same continuum covariance with respect to two different projections corresponding to different blocking kernels are of course different.

III.D.4 Comparison with the literature

To show that the work from the papers [128–131] is indeed original, we must make a comparison to how renormalisation was treated in the literature earlier on. The mainstream focused of course on the path integral renormalisation based on seminal work by Wilson, Bell and Hasenfratz et. al. using the example of the massless 2-dimensional Klein-Gordon field and the averaging blocking kernel [106, 112–114]. Their methods are quoted below, once for their own applications and afterwards for their applications in [130], where one considered for the first time also the deleting blocking kernel introduced in the last subsection.

We start with the Euclidian action for free massless scalar field in $d = 1+1$:

$$S := \frac{\beta}{2}\int_{\mathbb{R}^{D+1}} dt d^D x[\frac{1}{c}\dot\Phi^2 - c\Phi\omega^2\Phi] =: \frac{\beta}{2}\int d^dx\ \Phi G^2\Phi$$

and a discretisation thereof ($\epsilon_M := 1/M$):

$$S_M(\phi_M) =: \frac{\beta\epsilon_M^2}{2}\sum_{n\in\mathbb{Z}_M^2}\sum_{m\in\mathbb{Z}_M^2}\Phi_M(m)G_M^2(m,n)_M\Phi_M(n) \tag{III.271}$$

where M is the UV cut-off, that is, we consider a periodic lattice of unit length in each spacetime direction. The discretisation is translation- and reflection invariant $G_M^2(m,n) = G_M^2(||m-n||)$. The transformation of Euclidian actions

$$C\cdot e^{-\beta S'_M(\Phi_M)} := \int(\prod_m d\tilde\Phi_{2M}(m))e^{-\beta S_{2M}(\tilde\Phi_{2M})}e^{-2\kappa\sum_{n\in\mathbb{Z}_M^2}(\Phi_M - \frac{1}{4}\sum_{n'\in\mathbb{Z}^2_{2M}, n=\lfloor n'/2\rfloor)}\tilde\Phi_{2M})^2} \tag{III.272}$$

defines the approximate block spin transformation, where C is some unimportant, Φ_M-independent constant and the exponential on the right hand side is called the *averaging blocking kernel* that relates the fields Φ_M on the coarser lattice to those Φ_{2M} on the finer. In the limit $\kappa\to\infty$ the kernel becomes an exact Dirac δ Distribution, which fixes the new Φ_M to be an average of all the fields in the old block.

The action is diagonalised using the discrete Fourier transform: $\Phi_M(m) =: \frac{1}{M^2}\sum_l e^{ik_M l\cdot m}\hat\Phi_M(l)$ and $G_M^2(r) =: \frac{1}{M^2}\sum_l e^{ik_M l\cdot r}\hat G_M^2(l)$, with $k_M := \frac{2\pi}{M}$, $l\in\mathbb{Z}_M^2$. We obtain

$$\epsilon_M^2\sum_{n,m\in\mathbb{Z}_M^2}\Phi_M(m)G_M^2(m,n)\Phi_M(n) = \epsilon_M^4\sum_{l\in\mathbb{Z}_M^2}\hat\Phi_M(l)\hat G_M^2(l)\hat\Phi_M(-l) \tag{III.273}$$

In the literature [106] one considers the Hamiltonian $H(\phi) = \frac{1}{2}\int dx\phi(-\Delta)\phi$ and plugs its discretisation straightforwardly into (III.272).

Averaging Blocking Kernel

This is a recapitulation of the strategy from the literature introduced by [106] and refined in [114]. In order to find the fixed point, one studies the generating functional $Z(\beta J)$ of $J\in L_M$

$$\begin{aligned} Z(\beta J) &= \frac{1}{Z}\int d\Phi_M e^{-\frac{\beta}{2}\epsilon_M^2\sum_{m,n\in\mathbb{Z}_M^2}\Phi_M(m)G_M^2(m-n)\Phi_M(n)}e^{\beta\epsilon_M^2\sum_{n\in\mathbb{Z}_M^2}J_M(n)\Phi_M(n)} \\ &= \frac{1}{Z}\int d\hat\Phi_M e^{-\frac{\beta}{2}\epsilon_M^4\sum_{l\in\mathbb{Z}_M^2}\hat\Phi_M(l)\hat G_M^2(l)\hat\Phi_M(-l)+\beta\epsilon_M^4\hat J_M(-l)\hat\Phi_M(l)} \end{aligned} \tag{III.274}$$

with Z being the partition function and $d\Phi_M$ is the M^2- dimensional Lebesgue measure. In a first step, one shifts the variables

$$\hat{\Phi}_M(l) = \frac{\hat{J}_M(l)}{\hat{G}^2_M(l)} + \hat{\chi}_M(l) \tag{III.275}$$

such that the integral over the $\hat{\chi}_M$ can be computed and cancels the factor $1/Z$:

$$\begin{aligned} Z(\beta J) &= \frac{1}{Z}\int d\hat{\chi}_M \exp\left(-\frac{\beta}{2}\epsilon^4_M \sum_{l\in\mathbb{Z}^2_M} \hat{\chi}_M(l)\hat{G}^2_M(l)\hat{\chi}_M(-l) + \frac{3\beta}{2}\epsilon^4_M \sum_{l\in\mathbb{Z}^2_M} \frac{\hat{J}_M(l)\hat{J}_M(-l)}{\hat{G}^2_M(l)}\right) = \\ &= \exp\left(\frac{3}{2}\beta\epsilon^4_M \sum_{l\in\mathbb{Z}^2_M} \frac{\hat{J}_M(l)\hat{J}_M(-l)}{\hat{G}^2_M(l)}\right) \end{aligned} \tag{III.276}$$

If we expand this expression and (III.274) both to second order in $\hat{J}_M$, we get:

$$\begin{aligned} &\frac{(\beta\epsilon^4_M)^2}{Z} \sum_{l,l'\in\mathbb{Z}^2_M} \hat{J}_M(-l)\hat{J}_M(-l)\int d\hat{\phi}_M \hat{\Phi}_M(l)\hat{\Phi}_M(l')\exp\left(-\frac{\beta}{2}\epsilon^4_M \sum_{l_2\in\mathbb{Z}^2_M} \hat{\Phi}_M(l_2)\hat{G}^2_M(l_2)\hat{\Phi}_M(-l_2)\right) \\ &= \frac{3}{2}\beta\epsilon^4_M \sum_{l\in\mathbb{Z}^2_M} \hat{J}_M(l)\hat{J}_M(-l)\frac{1}{\hat{G}^2_M(l)} \end{aligned} \tag{III.277}$$

Since this expression holds for all $\hat{J}_M$ it follows

$$\frac{1}{Z}\int d\hat{\Phi}_M \hat{\Phi}_M(l)\hat{\Phi}_M(l')e^{-\frac{\beta}{2}\epsilon^4_M \sum_{l_2\in\mathbb{Z}^2_M} \hat{\Phi}_M(l_2)\hat{G}^2_M(l_2)\hat{\Phi}_M(-l_2)} = \left(\frac{3}{2\beta\epsilon^4_M}\right)^{-1}\frac{\delta(l+l')}{\hat{G}^2_M(l)} \tag{III.278}$$

This can be used in order to compute the 2-pt-function, which we translate into Fourier space:

$$\begin{aligned} \langle\Phi_M(n)\Phi_M(n')\rangle &= \frac{1}{Z}\int d\Phi_M \Phi_M(n)\Phi_M(n')\exp(-\beta S_M(\Phi_M)) \\ &= \frac{M^{-4}}{Z}\sum_{l,l'\in\mathbb{Z}^2_M} e^{i(k_M ln + k_M l'n')}\int d\hat{\Phi}_M\hat{\Phi}_M(l)\hat{\Phi}_M(l')e^{-\frac{\beta}{2}\epsilon^4_M\sum_{l_2\in\mathbb{Z}^2_M}\hat{\Phi}_M(l_2)\hat{G}^2_M(l_2)\hat{\Phi}_M(-l_2)} \overset{(III.278)}{=} \\ &= \sum_{l,l'\in\mathbb{Z}^2_M} e^{ik_M(ln+l'n')}\delta(l+l')\frac{1}{\hat{G}^2_M(l)}\frac{3}{2\beta} = \\ &= \sum_{l\in\mathbb{Z}^2_M} e^{ik_M l(n-n')}\frac{1}{\hat{\Omega}^2_M(l)}\left(\frac{3}{2\beta}\right) \approx \int_{[0,2\pi]^2}\frac{d^2k}{(2\pi)^2}e^{ik(n-n')}\frac{1}{\epsilon^2_M\hat{G}^2_M(k)}\left(\frac{3}{2\beta}\right) \end{aligned} \tag{III.279}$$

The approximation in the last line becomes exact in the *continuum limit* $M\to\infty$ in which we may replace $k_M l = 2\pi l/M$ by $k\in[0,2\pi]$.

For the renormalisation flow defined by (III.272), we can compute the 2-pt-function of the coarser lattice in terms of the 2-pt-function on the finer lattice:

$$\langle\hat{\Phi}_M(n),\hat{\Phi}_M(n')\rangle_M = \tag{III.280}$$
$$= \frac{1}{Z}\int d\Phi_M\,(\Phi_M(n)\Phi_M(n'))\exp\left(-\frac{\beta}{2}\epsilon_M^2\sum_{m,m'\in\mathbb{Z}_M}\Phi_M(m)(G^2)'_M(m-m')\Phi_M(m')\right) =$$
$$= \frac{1}{ZC}\int d\Phi_M\,(\Phi_M(n)\Phi_M(n'))\int d\Phi_{2M}\exp\left(-2\kappa\sum_{m\in\mathbb{Z}_M^2}(\Phi_M(m)-\frac{1}{4}\sum_{m''\in\mathbb{Z}_{2M}^2, m=\lfloor m''/2\rfloor}\Phi_{2M}(m''))^2\right)$$
$$\times\exp\left(-\frac{\beta}{2}\epsilon_{2M}^2\sum_{m,m'\in\mathbb{Z}_{2M}^2}\Phi_{2M}(m)G^2_{2M}(m-m')\Phi_{2M}(m)\right) =$$
$$= \frac{1}{ZC}\int d\Phi_{2M}\exp\left(-\frac{\beta}{2}\epsilon_{2M}^2\sum_{m',m''\in\mathbb{Z}_{2M}}\Phi_{2M}(m')G^2_{2M}(m'-m'')\Phi_{2M}(m'')\right)\times$$
$$\times\int d\Phi_M\,(\Phi_M(n)\Phi_M(n'))\exp\left(-2\kappa\sum_{m\in\mathbb{Z}_M}(\Phi_M(m)-\frac{1}{4}\sum_{m'\in\mathbb{Z}_{2M}, m=\lfloor m'/2\rfloor}\Phi_{2M}(m'))^2\right)$$

where we used (III.272) in the second step. Here the appearing integrals over $\Phi_M(\tilde{n})$ are all Gaussians (except for $\tilde{n}=n,n'$) and cancel with the constant C. The remaining give back the normalisation $\sqrt{\pi/(2\kappa)}$ twice for $n\neq n'$ and once if $n=n'$. Thus (III.280) becomes

$$= \frac{1}{Z}\int d\Phi_{2M}e^{-\beta S_{2M}(\Phi_{2M})}\left(\frac{2\kappa}{\pi}(1-\delta_{n,n'})\sum_{m,m'\in\mathbb{Z}_{2M}^2}\frac{1}{16}\Phi_{2M}(m)\Phi_{2M}(m')\left(\int d\phi e^{-2\kappa\phi^2}\right)^2+\right.$$
$$\left.+\sqrt{\frac{2\kappa}{\pi}}\delta_{n,n'}\frac{1}{16}\sum_{m,m'\in\mathbb{Z}_{2M}^2}\Phi_{2M}(m)\Phi_{2M}(m')\left(\int d\phi e^{-2\kappa\phi^2}\right)+\sqrt{\frac{2\kappa}{\pi}}\delta_{n,n'}\int d\phi\phi^2e^{-2\kappa\phi^2}\right)$$
$$= \frac{1}{16}\sum_{m,m'\in\mathbb{Z}_{2M}^2, n=\lfloor m/2\rfloor, n'=\lfloor m'/2\rfloor}\langle\hat{\Phi}_{2M}(n)\hat{\Phi}_{2M}(n')\rangle_{2M}+\frac{1}{4\kappa}\delta_{n,n'} \tag{III.281}$$

Iterating this transformation $j-$times yields

$$\langle\hat{\Phi}_M(n)\hat{\Phi}_M(n')\rangle_M = \tag{III.282}$$
$$= \left(\frac{1}{4}\right)^{2j}\sum_{m,m'\in\mathbb{Z}_{2^jM}^2, n=\lfloor m/2^j\rfloor, n'=\lfloor m'/2^j\rfloor}\langle\hat{\Phi}_{2^jM}(n)\hat{\Phi}_{2^jM}(n')\rangle_{2^jM}+\frac{1}{4\kappa}(1+\frac{1}{4}+\frac{1}{4^2}+\ldots+\frac{1}{4^{j-1}})\delta_{n,n'}$$

Simultaneous with the limit $j\to\infty$, we consider the original lattice to become infinitely fine, such that the summations in the first term on the right-hand side go over to integrals for which we must absorb the factor 2^{-j}.

Moreover, it is assumed safe in [114] to perform the limit of the 2-pt function separately and plug in the standard $\frac{1}{p^2}$ propagator for the infinitely fine lattice. Following their strategy, we arrive for large j at

$$\langle\hat{\Phi}_M(n)\hat{\Phi}_M(n')\rangle \approx \int_{-1/2}^{1/2}d^2x\int_{-1/2}^{1/2}d^2x'\left(\int_{-\infty}^{\infty}\frac{d^2p}{(2\pi)}\frac{e^{ip\cdot(n+x-n'-x')2\epsilon_M}}{p^2}\right)+\frac{1}{3\kappa}\delta_{n,n'} \tag{III.283}$$

Now we compare (III.283) with (III.279) - which was the 2-pt function at a fixed point - by diving the p_i integration into a summation of the integer l_i and an integration over k_i, i.e. $p=k+2\pi l$ such that:

$$\int_{-\pi}^{\pi}\frac{d^2k}{(2\pi)^2}e^{ik(n-n')}\frac{1}{\hat{G}_M^2(k)}\frac{3}{2\beta\epsilon_M^2} =$$
$$= \int_0^{2\pi}\frac{d^2k}{(2\pi)^2}\sum_{l\in\mathbb{Z}^2}\frac{1}{(k+2\pi l)^2}\int_{1/2}^{-1/2}dx\int_{1/2}^{-1/2}dx'e^{i(k+2\pi l)(n+x-n'-x')}+\int_{-\pi}^{\pi}\frac{d^2k}{2\pi}e^{ik(n-n')}\frac{1}{3\kappa} \tag{III.284}$$

It follows:

$$\frac{1}{\epsilon_M^2 \hat{G}_M^2(k)} = \frac{2\beta}{9\kappa} + \sum_{l\in\mathbb{Z}^2} \frac{2\beta/3}{(k+2\pi l)^2} e^{i2\pi l(n-n')} \frac{(-1)}{(k/2+\pi l)^2} \frac{\left[e^{i(k+2\pi l)x}\right]_{-1/2}^{1/2}}{2i} \frac{\left[e^{-i(k+2\pi l)x'}\right]_{-1/2}^{1/2}}{2i} =$$

$$= \sum_{l\in\mathbb{Z}^2} \frac{2\beta/3}{(k+2\pi l)^2} \prod_{\mu=0}^{1} \frac{\sin(k_\mu/2+\pi l_\mu)^2}{(k_\mu/2+\pi l_\mu)^2} + \frac{2\beta}{3\kappa} \tag{III.285}$$

This is the final expression for the covariance at the fixed point as found in the literature.

Deleting Blocking Kernel

Now, we repeat the analysis of the previous paragraph for the deleting kernel

$$e^{-2\kappa \sum_{m'\in\mathbb{Z}_M^2}(\Phi_M(m)-\Phi_{2M}(2m))^2} \tag{III.286}$$

In the previous section it was applied only in the spatial direction, but in order to relate with the literature we will use it here in the covariant context.

We compute the flow defined by this kernel by looking again at the 2-pt-function on a coarse lattice in terms of the 2-pt-function on the finer lattice:

$$\begin{aligned}
&\langle\hat{\Phi}_M(n)\hat{\Phi}_M(n')\rangle_M = \\
&= \frac{1}{Z}\int d\Phi_M \left(\Phi_M(n)\Phi_M(n')\right) \exp\left(-\frac{\beta}{2}\epsilon_M^2 \sum_{m,m'\in\mathbb{Z}_M^2} \Phi_M(m)(G^2)'_M(m-m')\Phi_M(m')\right) = \\
&= \frac{1}{Z\cdot C}\int d\Phi_M \left(\Phi_M(n)\Phi_M(n')\right)\int d\Phi_{2M}\times \\
&\quad\times \exp\left(-2\kappa \sum_{m\in\mathbb{Z}_M^2}(\Phi_M(m)-\Phi_{2M}(2m))^2 - \frac{\beta}{2\epsilon_M}\sum_{m,m'\in\mathbb{Z}_{2M}^2}\Phi_{2M}(m)G_{2M}^2(m-m')\Phi_{2M}(m')\right) \\
&= \frac{1}{Z\cdot C}\int d\Phi_{2M} \exp\left(-\frac{\beta}{2\epsilon_M}\sum_{m,m'\in\mathbb{Z}_{2M}^2}\Phi_{2M}(m)G_{2M}^2(m-m')\Phi_{2M}(m')\right)\times \\
&\quad\times \int d\Phi_M \left(\Phi_M(n)\Phi_M(n')\right)\exp\left(-2\kappa\sum_{m\in\mathbb{Z}_M^2}(\Phi_M(m)-\Phi_{2M}(2m))^2\right)
\end{aligned} \tag{III.287}$$

where we used (III.286) in the second step. The integrals over $\Phi_{2M}(m)$ are all Gaussian, except for $m = n, n'$, and cancel with the constant C. The remaining integrals return two or one factors of the normalisation $\sqrt{\pi/(2\kappa)}$ and (III.287) becomes

$$\begin{aligned}
&= \frac{1}{\left(\frac{\pi}{2\kappa}\right) Z}\int d\Phi_{2M} e^{-\beta S_{2M}(\Phi_{2M})}\Bigg((1-\delta_{n,n'})\prod_{i=n,n'}\int d\Phi_M(i)\,\times \\
&\quad\times\left(\Phi_M(i)-\Phi_{2M}(2i)+\Phi_{2M}(2i)\right)e^{-2\kappa\sum_{i=n,n'}(\Phi_M(i)-\Phi_{2M}(2i))^2} + \\
&\quad+\delta_{n,n'}\sqrt{\frac{\pi}{2\kappa}}\int d\Phi_M(n)\left(\Phi_M(n)-\Phi_{2M}(2n)+\Phi_{2M}(2n)\right)^2 e^{-2\kappa(\Phi_M(n)-\Phi_{2M}(2n))^2}\Bigg) \\
&= \langle\hat{\Phi}(2n)\hat{\Phi}(2n')\rangle_{2M} + \frac{1}{4\kappa}\delta_{n,n'}
\end{aligned} \tag{III.288}$$

After j steps of iteration

$$\langle\hat{\Phi}_M(n)\hat{\Phi}_M(n')\rangle^{(j)} = \langle\hat{\Phi}_{2^jM}(2^jn)\hat{\Phi}_{2^jM}(2^jn')\rangle + \frac{j}{4\kappa}\delta_{n,n'} \tag{III.289}$$

In the limit $j\to\infty$ the last term is problematic unless we take first the limit $\kappa\to\infty$. Note that $\Phi_{2^jM}(2^jn) = \Phi(2^jn\epsilon_{2^jM}) = \Phi(n\epsilon_M)$ in terms of the continuum field. For the 2-pt-function in the continuum we take the standard $1/p^2$ propagator. In total

$$\langle\hat{\Phi}_M(n)\hat{\Phi}_M(n')\rangle_M = \int_{-\infty}^{\infty}\frac{dp}{(2\pi)}\frac{1}{p^2}e^{ip(n+\frac{1}{2}-n'-\frac{1}{2})(2\epsilon_M)} \tag{III.290}$$

Now we compare this to (III.279) by diving the p integration again into a summation of the integer l and an integration over k, i.e. $p = k + 2\pi l$, whence

$$\int_{\pi}^{\pi}\frac{dk}{2\pi}e^{ik(n-n')}\frac{1}{\hat{G}_M^2(k)}\left(\frac{3}{2\beta\epsilon_M^2}\right) = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\sum_{l\in\mathbb{Z}_M^2}\frac{2\epsilon_M}{(k+2\pi l)^2}e^{i(k+2\pi l)(n-n')} \tag{III.291}$$

$$\Rightarrow \frac{1}{\epsilon_M^2\hat{G}_M^2} = \sum_{l\in\mathbb{Z}_M^2}\frac{2\beta/3}{(k+2\pi l)^2} \tag{III.292}$$

We see that the determining equation for $\hat{G}_M$ looks different than in case of the averaging blocking kernel. This was to be expected, since, to the best of our knowledge, there are no indication that the universality properties of the renormalisation group should improve, when considered in the covariant setting. The advantage of the deleting blocking kernel over the averaging blocking kernel, which has been considered e.g. in [114], is that it presents a cylindrically consistent fixed point. The averaging blocking kernel is only consistent if we perform the limit $\kappa \to \infty$.
In summary, in the case of the free field the search for a fixed point of the renormalisation group flow could be finished analytically in the covariant setting. However, an immediate drawback of the strategy here is that it requires explicit knowledge of continuum 2-pt function, e.g. in (III.283). For the application we have in mind, this information will in general be not available and we would rather follow the strategy of the direct Hamiltonian renormalisation as discussed in subsection *III.C.4 Direct Hamiltonian Renormalisation*.

III.D.5 Perfect Lattice Laplacian

The adjective "perfect" is used in renormalisation theory in order to characterise quantities at finite resolution of the fixed point theory. For instance, the family of fixed point covariances labelled by the finite resolution (lattice) parameter M in the free field theory case defines an effective covariance which can be interpreted as the result of integrating the spacetime Weyl element against the exponential of an effective action at the given resolution. This action is called "perfect action", actually a whole family thereof. In this section we investigate the family of "perfect Laplacians" which can be extracted from the family of fixed point covariances and study the decay behaviour of the contribution of lattice points in r-th neighbour relation to a given lattice point.

To avoid confusion, in the literature the term "perfect lattice Laplacian" mostly refers to the Euclidian d'Alembert operator, i.e. the operator $\Box = \partial_t^2 + \Delta$ involving time where Δ is the spatial Laplacian. In our case, we are more interested in the "perfect spatial lattice Laplacian" which refers to Δ. These two quantities are defined in terms of the finite resolution operators given by the fixed point theory. We have direct access to the fixed point family of spacetime covariances

$$M \mapsto C_M^* := (1_{L_2}\otimes I_M)^\dagger(p^2-\Box)^{-1}(1_{L_2}\otimes I_M) \tag{III.293}$$

of our renormalisation flow whose Fourier transforms $\hat{C}_M^*(k_0,l),\ l\in\mathbb{Z}_M$ were explicitly computed. We can now define the perfect Euclidian d'Alembertian as $-\Box_M^* := (C_M^*)^{-1} - p^2$. Recall the continuum covariance (dropping all prefactors, $\epsilon_M = \frac{R}{M}$, $k_M = \frac{2\pi}{M}$)

$$C = \frac{1}{2}(-\partial_t^2 - \Delta + p^2)^{-1} \tag{III.294}$$

The initial datum for the RG-flow was defined in terms of the naively discretised Laplacian, i.e. $(\Delta_M^{(0)}f_m)(m) = (f_M(m+1)+f_M(m-1)-2f_M(m))/\epsilon_M^2$, with covariance

$$C_M^{(0)} = \frac{1}{2}(-\partial_t^2 - \Delta_M^{(0)} + p^2)^{-1} \tag{III.295}$$

Its flow in Fourier space gave the fixed point

$$\frac{2}{\epsilon_M^2}\hat{C}_M^*(k_0,l) = \frac{1}{q^3}\frac{(\cosh(q)q-\sinh(q)+(\sinh(q)-q)\cos(t))}{\cosh(q)-\cos(t)} \tag{III.296}$$

with $t = k_M, q^2 = (k_0^2 + p^2)\epsilon_M^2$. The Fourier transform of the perfect d'Alembertian family $M \mapsto \Box_M^*$ is given by the inverse of (III.295):

$$-\hat{\Box}_M^* + p^2 := \epsilon_M^{-2} \frac{q^3[\mathsf{ch}(q) - \cos(t)]}{\mathsf{ch}(q)q - \mathsf{sh}(q) + (\mathsf{sh}(q) - q)\cos(t)} \tag{III.297}$$

The partially discrete kernel $(\Box_M^* F_M)(s,m) =: \int ds' \sum_{m' \in \mathbb{Z}_M} \Box_M^*(s-s', m-m') F_M(s', m')$ reads explicitly

$$\Box_M^*(s,r) = \int \frac{dk_0}{2\pi} \frac{1}{M} \sum_{l \in \mathbb{Z}_M} e^{ik_M lr + isk_0} [p^2 - \epsilon_M^{-2} \frac{q^3[\mathsf{ch}(q) - \cos(t)]}{\mathsf{ch}(q)q - \mathsf{sh}(q) + (\mathsf{sh}(q) - q)\cos(t)}] \tag{III.298}$$

We want to find out whether that $\Box_M^*(s,r)$ decays exponentially fast with the spatial neighbour parameter r. To do this, we define the forward and backward lattice shifts as follows

$$(\delta^{+k} f)(m) = f(m+k), \qquad (\delta^{-k} f)(m) = f(m-k) \tag{III.299}$$

with $k = -\lfloor M/2 \rfloor, ..., \lfloor M/2 \rfloor$ which implies $(\delta^+)^n = \delta^{+n}$ and $\delta^+\delta^- = \delta^-\delta^+$. Note that $\delta^{\pm k + \alpha M} = \delta^{\pm k}$ for all $\alpha \in \mathbb{Z}$.

Now $\cos(t)$ is an eigenvalue of $\mathfrak{d} := [\delta^+ + \delta^-]/2$ in Fourier space

$$(\mathfrak{d} e^{it\cdot})(m) = \frac{1}{2}(e^{itm+it} + e^{itm-it}) = cos(t) e^{itm} \tag{III.300}$$

so that

$$\Box_M^*(s,r) = \int \frac{dk_0}{2\pi} e^{isk_0} \left([p^2 - \epsilon_M^{-2} \frac{q^3[\mathsf{ch}(q) - \mathfrak{d}]}{\mathsf{ch}(q)q - \mathsf{sh}(q) + (\mathsf{sh}(q) - q)\mathfrak{d}}] \cdot {}^K\delta_0\right)(r) \tag{III.301}$$

where $r \mapsto {}^K\delta_{0,r} \equiv {}^K\delta(0,r)$ is the Kronecker δ supported at 0 and the operator $\mathfrak{d}$ acts on the variable r in this formula. Similarly, we may introduce the operator $Q^2 := \epsilon_M^2(p^2 - \partial_s^2)$ and the function $A(Q) := (\mathsf{sh}(Q) - Q)/(Q\mathsf{ch}(Q) - \mathsf{sh}(Q))$. Then

$$\epsilon_M^2 \Delta_M^*(s,r) := \epsilon_M^2(\Box_M^* - \partial_s^2)(s,r) = \left([Q^2 - \frac{Q^3}{Q\mathsf{ch}(Q) - \mathsf{sh}(Q)} \frac{\mathsf{ch}(Q) - \mathfrak{d}}{1 + A(Q)\mathfrak{d}}] \cdot \delta_0 \otimes {}^K\delta_0\right)(s,r) \tag{III.302}$$

where δ_0 is the Dirac δ distribution for the temporal degree of freedom.
The first term in (III.302) gives a contribution on $r = 0$ only. Hence, to study the decay behaviour for spatial directions, we focus on the second term: By integrating respectively summing (III.301) against time-independent functions $f(s,r) = f_M(r), f'(s',r') = f'_M(r')$ we obtain $\delta_{k_0,0}$, in other words $Q^2 = q_0^2 := p^2\epsilon_M^2$ and

$$\langle f', \Box_M^* f \rangle = \langle f'_M, \Delta_M^* f_M \rangle_M \tag{III.303}$$

The idea is now to expand its denominator into a geometric series with respect to the operator $\mathfrak{d}$ and to extract the coefficients of $\delta^{\pm k}$. To expand it into a Neumann-series, we must check for convergence of the series. This will be guaranteed if $||A(q_0)\mathfrak{d}|| \leq 1$ in the operator norm $||.||$.
First, note that $A(q_0) \leq \frac{1}{2}$ for all $q_0 \geq 0$, because

$$\begin{aligned} 2(\mathsf{sh}(q_0) - q_0) \leq q_0\mathsf{ch}(q_0) - \mathsf{sh}(q_0) \;&\Leftrightarrow \\ 3\mathsf{sh}(q_0) \leq q_0\mathsf{ch}(q_0) + 2q_0 \;&\Leftrightarrow \\ \sum_k \frac{3}{(2n+1)!} q_0^{2n+1} \leq \sum_k \frac{1}{(2n)!} q_0^{2n+1} + 2q_0 & \end{aligned} \tag{III.304}$$

which can be checked by comparing all powers of q_0 separately.
Since $\delta^\pm$ are norm preserving, we use the Cauchy-Schwarz inequality to see that $||\mathfrak{d}|| \leq 1$. Thus, on the functions of independent time support

$$||A(q_0)\mathfrak{d}|| = |A(q_0)| \cdot ||\mathfrak{d}|| \leq 1/2 \tag{III.305}$$

and we can expand (III.302) into a geometric series.
This gives

$$\frac{\mathsf{ch}(q_0)-\mathfrak{d}}{1+A(q_0)\mathfrak{d}} = (\mathsf{ch}(q_0)-\mathfrak{d})\sum_{N=0}^{\infty}(-\mathfrak{d}A(q_0))^N = \sum_{N=0}^{\infty}(-A(q_0))^N\left(\mathsf{ch}(q_0)2^{-N}[\delta^+ + \delta^-]^N - 2^{-N-1}[\delta^+ + \delta^-]^{N+1}\right) =$$
$$= \sum_{N=0}^{\infty}(-A(q_0)/2)^N\left(\mathsf{ch}(q_0)\sum_{k=0}^{N}\binom{N}{k}\delta^{+k}\delta^{-(N-k)} - \frac{1}{2}\sum_{k=0}^{N+1}\binom{N+1}{k}\delta^{+k}\delta^{-(N+1-k)}\right) =$$
$$= \sum_{r\in\mathbb{Z}}\delta^{+2r}\left(\mathsf{ch}(q_0)\sum_{n=0}^{\infty}\binom{2n}{n+r}(-A(q_0)/2)^{2n} - \frac{1}{2}\sum_{n=1}^{\infty}\binom{2n}{n+r}(-A(q_0)/2)^{2n-1}\right) +$$
$$+ \sum_{r=1}^{\infty}\delta^{+2r-1}\left(\mathsf{ch}(q_0)\sum_{n=0}^{\infty}\binom{2n+1}{n+r}(-A(q_0)/2)^{2n+1} - \frac{1}{2}\sum_{n=0}^{\infty}\binom{2n+1}{n+r}(-A(q_0)/2)^{2n}\right) +$$
$$+ \sum_{r=1}^{\infty}\delta^{-2r+1}\left(\mathsf{ch}(q_0)\sum_{n=0}^{\infty}\binom{2n+1}{n-r+1}(-A(q_0)/2)^{2n+1} - \frac{1}{2}\sum_{n=0}^{\infty}\binom{2n+1}{n-r+1}(-A(q_0)/2)^{2n}\right) \tag{III.306}$$

where have chosen $2r := k-(N-k) \Rightarrow N =: 2n$ and $2r := k-(N+1-k) \Rightarrow N =: 2n-1$ respectively for the even powers of $\delta^{\pm}$ and similar for the odd contributions. During this procedure, we used Fubini's theorem to exchange the summation order of r, n.
Indeed, for $A(q) \leq 1/2$ each sum over n converges separately:

$$\sum_{n=0}^{\infty}\binom{2n}{n+r}\cdot(A(q)/2)^{2n} \leq \sum_{n=0}^{\infty}\frac{(2n)^{n+r}}{(n+r)!}\cdot 4^{-2n} \leq \sum_{n=0}^{\infty}\frac{4^{-2n}}{e}\left(\frac{2n\,e}{(n+r)}\right)^{n+r} =$$
$$= \sum_{n=0}^{\infty}2^r e^{r-1}\left(\frac{1}{1+r/n}\right)^{n+r}\left(\frac{e}{8}\right)^n \leq \sum_{n=0}^{\infty}2^r e^{r-1}\left(\frac{e}{8}\right)^n = \frac{2^{r+3}e^{r-1}}{8-e} \tag{III.307}$$

where we have used a standard approximation for the factorial, i.e. $(n/e)^n e \leq n!$, and summed a geometric series. Thus, the inner sums over n in (III.306) are finite. The convergence and

$$\sum_{n=0}^{\infty}\binom{2n}{n+r}z^{2n} = \sum_{n=0}^{\infty}\binom{2n}{n-r}z^{2n} = \sum_{k=0}^{\infty}\binom{2k+2r}{k}z^{2k+2r} \tag{III.308}$$

allow to identify the series with a *generalised binomial series* $\mathcal{B}_t(z)$. These kinds of sums were introduced by Lambert in 1758 [217] and he showed later that its powers $r \in \mathbb{Z}$ obey the following property [218]

$$\mathcal{B}_t(z)^r = \sum_{k=0}^{\infty}\binom{tk+r}{k}\frac{r}{tk+r}z^k \tag{III.309}$$

$\forall t \in \mathbb{Z}$ and $z \in \mathbb{R}$ such that the series converges. A modern proof of this statement can be found in [219]. Further, we quote the following identities from [220]

$$\frac{\mathcal{B}_2(z)^r}{\sqrt{1-4z}} = \sum_{k=0}^{\infty}\binom{2k+r}{k}z^k, \qquad \mathcal{B}_2(z) = \frac{1-\sqrt{1-4z}}{2z} \tag{III.310}$$

Using this, we can compute the series explicitly: Let $s \in \{0,1\}$

$$\sum_{n=0}^{\infty}\binom{2n+s}{n+r}(-A(q_0)/2)^{2n} = \sum_{k=0}^{\infty}\binom{2k+2r-s}{k}(A(q_0)/2)^{2k}(A(q_0)/2)^{2r-2s} =$$
$$= \frac{(A(q_0)/2)^{2r-2s}}{\sqrt{1-4(A(q_0)/2)^2}}\mathcal{B}_2(A(q_0)^2/4)^{2r-s} = \frac{(A(q_0)/2)^{2r-2s}}{\sqrt{1-A(q_0)^2}}\left(\frac{2}{A(q_0)^2}\right)^{2r-s}(1-\sqrt{1-A(q_0)^2})^{2r-s} =$$
$$= \frac{2^s(1-\sqrt{1-A(q_0)^2})^{-s}}{\sqrt{1-A(q_0)^2}}\left(\frac{1-\sqrt{1-A(q_0)^2}}{A(q_0)}\right)^{2r} \sim \exp\left(r\cdot 2\log[1/A(q_0)-\sqrt{1/A(q_0)^2-1}]\right) =: e^{r\Theta(q_0)} \tag{III.311}$$

For finite q_0, we have $0 < A(q_0) \leq 1/2$ and the logarithm is always well-defined and negative, since it holds that $1 - \sqrt{1 - A(q_0)^2} \leq A(q_0)$.
Thus, the perfect spatial lattice Laplacian is on the subspace of functions of independent time support explicitly given by

$$\begin{aligned}\epsilon_M^2 \Delta_M^* =& (q_0^2 + \frac{q_0^3 A(q_0)^{-1}}{q_0 \mathsf{ch}(q_0) - \mathsf{sh}(q_0)})\, \mathbb{1} - \\ &- \frac{q_0^3 \sqrt{1 - A(q_0)^2}^{-1}}{q_0 \mathsf{ch}(q_0) - \mathsf{sh}(q_0)} (\mathsf{ch}(q_0) A(q_0) + 1) \cdot \left(\sum_{r \in \mathbb{Z}} \delta^{+2r} \frac{e^{|r| \Theta(q_0)}}{A(q_0)} - \sum_{r=1}^{\infty} (\delta^{+(2r-1)} + \delta^{-(2r-1)}) \frac{e^{|r|\Theta(q_0)}}{1 - \sqrt{1 - A(q_0)^2}} \right)\end{aligned} \tag{III.312}$$

Lastly, we must account for the periodic boundary conditions. Remembering that the lattice identifies the points r and $r + \alpha M$ with $\alpha \in \mathbb{Z}$, we add all corresponding contributions together. For the even powers of the shift operator:

$$\sum_{r \in \mathbb{Z}} \delta^{2r} e^{|r|\Theta(q_0)} = \sum_{r=-\lfloor M/4 \rfloor}^{\lfloor M/4 \rfloor} \delta^{2r} e^{|r|\Theta(q_0)} \sum_{\alpha \in \mathbb{Z}} e^{M|\alpha|\Theta(q_0)} = \sum_{r=-\lfloor M/4 \rfloor}^{\lfloor M/4 \rfloor} \delta^{2r} e^{|r|\Theta(q_0)} [\frac{2}{1 - (\frac{1}{A(q_0)} - \sqrt{\frac{1}{A(q_0)^2} - 1})^{2M}} - 1]$$

and the same geometric sum appears for the odd powers. For big lattices, i.e. $M >> 1$, we see that due to $0 < A(q_0) \leq 1/2$ the term in the brackets [...] approaches 1 very fast.
In total, we conclude that the perfect spatial Laplacian decays exponentially with r and has a damping factor of $\Theta(q_0 = p\epsilon_M^2)$. So, although it features non-local contributions, these are highly suppressed.

III.E Example: Klein Gordon field III - Rotational Invariance

Along the lines of [131] we will now study the natural extension of the toy model "Klein Gordon field" from the previous sections to multiple dimensions. Hence, we keep the general action:

$$S := \frac{1}{2\kappa}\int_{\mathbb{R}^{D+1}} dt d^D x [\frac{1}{c}\dot{\phi}^2 - c\phi\omega\phi] \tag{III.313}$$

with $(n = 1, 2, ..)$

$$\omega^2 = \omega^2(p, \Delta) = \frac{1}{p^{2(n-1)}}(-\Delta + p^2)^n \tag{III.314}$$

where $p = \frac{mc}{\hbar}$ is the inverse Compton length. Following [129] we will study here the Poincare invariant case with $n = 1$, other models with $n \neq 1$ can be studied with the methods developed for $n = 1$ by contour integral techniques.

After performing the Legendre transform, introducing the IR cut-off and discretising the theory for various resolutions M, one considers the lattice Hamiltonian family ($\hbar = 1$)

$$H_M := \frac{c}{2}\sum_{m\in\mathbb{Z}_M^D}\left(\kappa\epsilon_M^D \pi_M^2(m) + \frac{1}{\kappa\epsilon_M^D}\phi_M(m)(\omega_M^2\cdot\phi_M)(m)\right) \tag{III.315}$$

with $(\pi := \dot{\phi}/\kappa)$

$$\phi_M(m) := \int_{[0,1)^D} d^D x \chi_{m\epsilon_M}(x)\phi(x), \qquad \pi_M(m) := (E_M\pi)(m) = \pi(m\epsilon_M) \tag{III.316}$$

and $\omega_M^2 = \omega^2(p, \Delta_M)$ is to be understood in terms of Δ_M the naively discretised Laplacian, which reads e.g. in two dimensions:

$$(\Delta_M^{(0)} f_M)(m) := \frac{1}{\epsilon_M^2}\left(f_M(m+e_1) + f_M(m+e_2) + f_M(m-e_1) + f_M(m-e_2) - 4f_M(m)\right) \tag{III.317}$$

with e_i being the unit vector in direction i. One can write down the explicit action of the coarse graining map for projecting a lattice on a finer version with twice as many lattice points:

$$(I_{M\to 2M} f_M)(m) = \sum_{m'\in\mathbb{Z}_M^D}\chi_{m'\epsilon_{2M}}(m\epsilon) f_M(m') = f_M(\lfloor\frac{m}{2}\rfloor) \tag{III.318}$$

where $\lfloor x\rfloor$ denotes the component wise Gauss bracket. According to the same argument as in the one dimensional case, the cylindrical consistency condition (III.58) demanded that the measures on both discretisation, M and $2M$, agree. Being a free field theory, one can show that the measure can be written as a Gaussian measure described at the fixed point by a covariance c_M^*, thus (III.58) reads explicitly

$$e^{-\frac{1}{2}\langle I_{M\to 2M} f_M, c_{2M}^* I_{M\to 2M} f_M\rangle_{2M}} = e^{-\frac{1}{2}\langle f_M, c_M^* f_M\rangle_M} \tag{III.319}$$

Thus by studying the flow defined by

$$c_M^{(n+1)} := I_{M\to 2M}^\dagger c_{2M}^{(n)} I_{M\to 2M} \tag{III.320}$$

we know that the existence of a fixed point c_M^* describes a Gaussian measure family, which is equivalent to corresponding Hilbert spaces $\mathcal{H}_M^*$ with vacua Ω_M^* which are all annihilated by the correspondingly defined Hamiltonians H_M^*.

III.E.1 Determination of the fixed point covariance

We quote the calculations from [131]. The flow defined by (III.320) may lead to various fixed points (or none at all) depending on the initial family $c_M^{(0)}$. Thus, the naive discretisation should be of such a form that it captures important features of the continuum theory. For example, we will demand the covariance to be translation invariant, which is a property of the discretised Laplacian and will remain true under each renormalisation

step.
We begin by rewriting (III.315) in terms of discrete annihilation and creation operators

$$a_M^{(0)}(m) := \frac{1}{\sqrt{2\hbar\kappa}}\left[\sqrt{\frac{\omega_M^{(0)}}{\epsilon_M^D}}\phi_M - i\kappa\sqrt{\frac{\epsilon_M^D}{\omega_M^{(0)}}}\pi_M(m)\right] \tag{III.321}$$

where

$$[\omega_M^{(0)}]^2 := p^2 - \Delta_M^{(0)} \tag{III.322}$$

which after some standard algebra displays the Hilbert space measure as:

$$\nu_M^{(0)}(w_M[f_M]) = \nu_M\left(e^{i\langle f_M,\phi_M\rangle_M}\right) = \exp\left(-\frac{1}{4}\langle f_M, \frac{\hbar\kappa}{2}\omega_M^{-1} f_M\rangle_M\right) \tag{III.323}$$

Hence our starting covariance is given as:

$$c_M^{(0)} = \frac{\hbar\kappa}{2}[\omega_M^{(0)}]^{-1} \tag{III.324}$$

Using the discrete Fourier transform ($k_M = \frac{2\pi}{M}$)

$$f_M(m) = \sum_{l\in\mathbb{Z}_M^D} \hat{f}_M(l)e^{ik_M l\cdot m}, \qquad \hat{f}_M(l) := M^{-D}\sum_{m\in\mathbb{Z}_M^D} f_M(m)e^{-ik_M m\cdot l} \tag{III.325}$$

we diagonalise the discretised Laplacian appearing in $\omega_M^{(0)}$. Thus, the initial covariance family becomes in $D=2$ (dropping the factor $\frac{2}{\hbar\kappa}$ in what follows)

$$\begin{aligned}\hat{c}_M^{(0)}(l) &= \frac{1}{\sqrt{-\frac{1}{\epsilon_M^2}(2\cos(k_M l_1) + 2\cos(k_M l_2) - 4) + p^2}} = \\ &= \int_{\mathbb{R}} \frac{dk_0}{2\pi}\frac{\epsilon_M^2}{[k_0^2+p^2]\epsilon_M^2 + (4 - 2\cos(k_M l_1) - 2\cos(k_M l_2))}\end{aligned} \tag{III.326}$$

with $l\in\mathbb{Z}_M^2$ and we used the residue theorem. We rewrite the integrand of (III.326) as ($t_i = k_M l_i, q^2 := (k_0^2+p^2)\epsilon_M^2$)

$$\hat{c}_M^{(0)}(k_0, l) = \frac{1}{2}\frac{\epsilon_M^2}{[q^2/4 + (1-\cos(t_1))] - [-q^2/4 - (1-\cos(t_2))]} \tag{III.327}$$

Since $1 + q^2/4 > \cos(t), \forall p > 0, t\in\mathbb{R}$ one deduces that the first of the square brackets in (III.327) is always positive, the other one always negative. Consequently, they lie in different halfplanes of $\mathbb{C}$. This can be used to artificially write this as an integral in the complex plane, by inverting the residue theorem: Given $z_1, z_2\in\mathbb{C}$ with $Re(z_1) > 0, Re(z_2) < 0$ and a curve γ going along $i\mathbb{R}$ from $+i\infty$ to $-i\infty$ and closing in the right plane on a half circle with radius $R\to\infty$, we can write:

$$\oint_\gamma dz\frac{1}{(z-z_1)(z-z_2)} = 2\pi i\frac{1}{z_1 - z_2} \tag{III.328}$$

since the integrand decays as z^{-2} on the infinite half circle. We have chosen the orientation of γ counter clock wise. Note that this seemingly breaks the symmetry between t_1 and t_2. However, this is only an intermediate artefact of the free choice of γ which will disappear at the end of the computation.

Substituting $z\to z/2$ the initial covariance can thus be written

$$\hat{c}_M^{(0)}(l) = -\oint_\gamma dz\frac{1}{8\pi i}\,\frac{\epsilon_M^2}{\epsilon_M^2(\frac{p^2+k_0^2}{2} - z)/2 + 1 - \cos(t_1)}\,\frac{\epsilon_M^2}{\epsilon_M^2(\frac{p^2+k_0^2}{2} + z)/2 + 1 - \cos(t_2)} \tag{III.329}$$

In order to shorten our notation, we will introduce: $q_{1,2}^2(z) := \epsilon_M^2([k_0^2+p^2]/2 \mp z)$. The starting point of our RG flow is now factorised into two factors which very closely resemble the 1+1 dimensional case. This is the promised factorising property.

Let us now focus on the precise action of the map (III.320), by writing it in terms of its kernel $c_M^{(n)}(m_1', m_2') = c_M^{(n)}(m_1' - m_2')$:

$$C_M^{(n+1)}(m_1' - m_2') = 2^{-2D}\sum_{\delta',\delta''\in\{0,1\}^D} C_{2M}^{(n)}(2m_1' + \delta' - 2m_2' + \delta'') \tag{III.330}$$

and correspondingly for the Fourier transform for $D=2$

$$\hat{c}_M^{(n+1)}(l) = 2^{-4} \sum_{\delta,\delta',\delta''\in\{0,1\}^2} \hat{c}_{2M}^{(n)}(l+\delta M) e^{ik_{2M}(l+\delta M)\cdot(\delta'-\delta'')} =$$

$$= \frac{1}{2^4} \sum_{\delta_1,\delta_2\in\{0,1\}} \hat{c}_{2M}^{(n)}(l_1+\delta_1 M, l_2+\delta_2 M) \Big(e^{ik_{2M}(l_1+l_2+(\delta_1+\delta_2)M)} + \\ + e^{-ik_{2M}(l_1+l_2+(\delta_1+\delta_2)M)} + e^{ik_{2M}(l_1-l_2+(\delta_1-\delta_2)M)} + e^{-ik_{2M}(l_1-l_2+(\delta_1-\delta_2)M)} \\ + 2e^{ik_{2M}(l_2+\delta_2 M)} + 2e^{-ik_{2M}(l_2+\delta_2 M)} + 2e^{ik_{2M}(l_1+\delta_1 M)} + 2e^{-ik_{2M}(l_1+\delta_1 M)} + 4 \Big) \tag{III.331}$$

where we wrote explicitly all 16 terms stemming from the different combinations of $(\delta'-\delta'')$.

$$= \frac{1}{2^4} \sum_{\delta_1,\delta_2=0,1} \hat{c}_{2M}^{(n)}(l_1+\delta_1 M, l_2+\delta_2 M) \left(4 + 4\cos(k_{2M}(l_2+\delta_2 M)) + 4\cos(k_{2M}(l_1+\delta_1 M)) + \\ + 2\cos(k_{2M}(l_1+\delta_1 M) + k_{2M}(l_2+\delta_2 M)) + 2\cos(k_{2M}(l_1+\delta_1 M) - k_{2M}(l_2+\delta_2 M))\right)$$
$$= \frac{1}{2^2} \sum_{\delta_1,\delta_2=0,1} \hat{c}_{2M}^{(n)}(l_1+\delta_1 M, l_2+\delta_2 M)\times \\ (1+\cos(k_{2M}(l_2+\delta_2 M)) + \cos(k_{2M}(l_1+\delta_1 M)) + \cos(k_{2M}(l_1+\delta_1 M))\cos(k_{2M}(l_2+\delta_2 M)))$$
$$= \frac{1}{4} \sum_{\delta_1,\delta_2=0,1} (1+\cos(k_{2M}(l_1+\delta_1 M)))(1+\cos(k_{2M}(l_2+\delta_2 M)))\, \hat{c}_{2M}^{(n)}(l_1+\delta_1 M, l_2+\delta_2 M) \tag{III.332}$$

where we have used in the second step, that $2\cos(x)\cos(y) = \cos(x+y) + \cos(x-y)$.

One realises that both directions completely decouple in the renormalisation transformation. Since the initial covariance factorises under the contour integral over γ this factorisation is preserved under the flow and implies that the flow of the covariance in each direction can be performed separately. At the end we then compute the resulting integral over z along γ. In addition, the decoupling of the flow (III.320) and the factorisation of the initial family of covariances (III.329) for the naive discretisation of the Laplacian are features that occur independently of the dimension D. For the decoupling this follows immediately from the corresponding generalisation of (III.331) as the sum over δ', δ'' is carried out on the exponential function which contains both linearly in the exponent. For the factorisation we note the following iterated integral identity for complex numbers $k_j,\ j=1,..,D$ with strictly positive real part

$$\frac{1}{k_1+..+k_D} = (2\pi i)^{D-1} \oint_\gamma \frac{dz_1}{z_1-k_1} \oint_\gamma \frac{dz_2}{z_2-k_2} .. \oint_\gamma \frac{dz_{D-1}}{z_{D-1}-k_{D-1}} \frac{1}{z_1+..+z_{D-1}+k_D} \tag{III.333}$$

in which γ is always the same closed contour with counter clock orientation over the half circle in the positive half plane followed by the integral over the imaginary axis. Because of that the real part of each of the integration variables z_j is non negative so that the last fraction has a denominator with strictly positive real part. Accordingly, the only pole of the integrand for the z_j integral in the domain bounded by γ is k_j and the claim follows from the residue theorem. It transpires that the strategy illustrated for the case $D=2$ also solves the case of general D and it therefore suffices to carry out the details for $D=2$.

The flow now acts on the integrand of the contour integral and we can do it for each z separately. The flow in each direction is thus described by exactly the same map as in the one dimensional case in [129]. We can therefore immediately copy the fixed point covariance from there. We just have to keep track of the z dependence. In direction $i=1,2$ the covariance can be parametrised by three functions of $q_i(z)$ ($t_i = k_M l_i$, $l_i \in \mathbb{Z}_M$)

$$\hat{c}_M^{(n)}(k_0, l_i, z) = \frac{\epsilon_M^2}{q_i^3(z)} \frac{b_n(q_i(z)) + c_n(q_i(z))\cos(t_i)}{a_n(q_i(z) - \cos(t_i)} \tag{III.334}$$

The initial functions are

$$a_0(q_{1,2}) = 1 + \frac{q_{1,2}^2}{2}, \qquad b_0(q_{1,2}) = \frac{q_{1,2}^3}{2}, \qquad c_0(q_{1,2}) = 0$$

Before plugging in the fixed points, however, one has to check whether the flow will drive the starting values into a finite fixed point, i.e. all the numerical prefactors that are picked up in front of the covariance should cancel each other. Indeed, one RG steps corresponds to

$$(2\pi i)\hat{c}_M^{(n+1)}(k_0,l) = -\frac{1}{4}\oint_\gamma dz \left(\sum_{\delta_1=0,1}(1+\cos(k_{2M}(l_1+\delta_1 M)))\hat{c}_{2M}^{(n)}(k_0,l_1,z)\right)\times$$
$$\times\left(\sum_{\delta_2=0,1}(1+\cos(k_{2M}(l_2+\delta_2 M)))\hat{c}_{2M}^{(n)}(k_0,l_2,-z)\right) \tag{III.335}$$

Note that $\epsilon_M \to \epsilon_{2M} = \epsilon_M/2$ whence

$$q_{1,2}^2 := \epsilon_M^2(\frac{p^2+k_0^2}{2} \mp z) \to \frac{1}{4}\epsilon_M^2(\frac{p^2+k_0^2}{2} \mp z) = q_{1,2}^2/4 \tag{III.336}$$

Collecting all powers of 2, we get 1. minus two from the ϵ_M^2 in the numerator of the factor for both directions, that is altogether minus four; 2. the RG map gives an additional minus two because of the $1/4$ prefactor; and 3. due to (III.336) the factor $q_1^{-3}q_2^{-3}$ gives a power of plus six. Hence the overall power of two is zero.

Accordingly, we find the same fixed points as in [129]:

$$a^*(q_{1,2}) = \mathsf{ch}(q_{1,2}) \tag{III.337}$$
$$b^*(q_{1,2}) = q_{1,2}\mathsf{ch}(q_{1,2}) - \mathsf{sh}(q_{1,2}) \tag{III.338}$$
$$c^*(q_{1,2}) = \mathsf{sh}(q_{1,2}) - q_{1,2} \tag{III.339}$$

where we write shorthand for the hyperbolic functions: $\mathsf{ch}(q) := \cosh(q)$ and $\mathsf{sh}(q) := \sinh(q)$. Thus we find with $t_j = k_M l_j$

$$\hat{c}_M^*(k_0,l) = -\left(\frac{\epsilon_M^4}{2\pi i}\right)\oint_\gamma dz \prod_{j=1,2}\frac{1}{q_j^3}\frac{q_j\mathsf{ch}(q_j) - \mathsf{sh}(q_j) + (\mathsf{sh}(q_j)-q_j)\cos(t_j)}{\mathsf{ch}(q_j)-\cos(t_j)} \tag{III.340}$$

Note that it is not necessary to pick a square root of the complex parameter $q_{1,2}^2(z) = \epsilon_M^2(\frac{k_0^2+p^2}{2} \mp z)$ since the integrand only depends on the square, despite its appearance (in other words, one may pick the branch arbitrarily, the integrand does not depend on it). It follows that the integrand is a single valued function of z which is holomorphic everywhere except for simple poles which we now determine, and which allow to compute the contour integral over γ using the residue theorem.

There are no poles at $q_{1,2}^2 = 0$ since the functions $[q\mathsf{ch}(q) - \mathsf{sh}(q)]/q^3,\ [\mathsf{sh}(q) - q]/q^3$ are regular at $q = 0$. Hence the only poles come from the zeroes of the function $\mathsf{ch}(q) - \cos(t)$. Using $\mathsf{ch}(iz) = \cos(z)$ and the periodicity of the cosine function we find $iq = \pm[t + 2\pi N]$ with $N \in \mathbb{Z}$ or $q^2 = -(t+2\pi N)^2$. In terms of $q_j,\ j = 1,2$ this means that

$$(k_0^2+p^2)/2 \mp z = -\frac{(t_j+2\pi N)^2}{\epsilon_M^2} \quad\Leftrightarrow\quad z = z_N = \pm[(k_0^2+p^2)/2 + \frac{(t_j+2\pi N)^2}{\epsilon_M^2}] \tag{III.341}$$

It follows that the second factor involving q_2 has no poles in the domain bounded by γ because they all lie on the negative real axis while those coming from the factor involving q_1 lie all on the positive real axis. We will denote the latter by z_N. The poles coming from the zeroes of $\mathsf{ch}(q_1) - \cos(t_1)$ are simple ones as one can check by expanding the hyperbolic cosine at z_N in terms of $z - z_N$, in other words

$$\lim_{z\to z_N}\frac{z-z_N}{\mathsf{ch}(q_1(z)) - \cos(t_1)} = \lim_{z\to z_N}\frac{1}{\mathsf{sh}(q_1(z))q_1'(z)} = \lim_{z\to z_N}\frac{2q_1(z)}{\mathsf{sh}(q_1(z))[q_1^2(z)]'} = -\frac{2q_1(z_N)}{\epsilon_M^2\mathrm{sh}(q_1(z_N))} \tag{III.342}$$

which is again independent of the choice of square root. We have used de l' Hospital's theorem in the second step. Note that $q_1(z_N)^2 = -(t_1+2\pi N)^2$ implies $q_2(z_N)^2 = q^2 + (t_1+2\pi N)^2 := q_N^2$ where $q^2 := \epsilon_M^2(k_0^2+p^2)$.

Performing the integral we finally end up with:

$$\hat{c}_M^*(l) = -2\epsilon_M^2\sum_{N\in\mathbb{Z}}\frac{\cos(t_1)-1}{(2\pi N+t_1)^3}(2\pi N+t_1)\times \tag{III.343}$$
$$\times\frac{\sqrt{q^2+(2\pi N+t_1)^2}[\mathsf{ch}(\sqrt{q^2+(2\pi N+t_1)^2}) - \cos(t_2)] + \mathsf{sh}(\sqrt{q^2+(2\pi N+t_1)^2})(\cos(t_2)-1)}{(q^2+(2\pi N+t_1)^2)^{3/2}[\mathsf{ch}(\sqrt{q^2+(2\pi N+t_1)^2}) - \cos(t_2)]]}$$

One sees that everything remains finite for $\epsilon \to 0$ as the individual parts contribute with inverse powers of ϵ_M: $(\cos(t)-1)$ goes with $\mathcal{O}(\epsilon_M^2)$, since $t = 2\pi\epsilon_M l$ depends linearly on ϵ_M. So does q and thus $(q^2+(t+2\pi N)^2) =$

$\mathcal{O}(\epsilon_M^2)$ if $N=0$ or a constant else.
We split the sum in the nominator of (III.343) in two parts. In first term we can explicitly compute the sum and obtain:

$$-2\sum_{N\in\mathbb{Z}}\frac{(\cos(t)-1)}{(2\pi N+t)^2(q^2+(2\pi N+t)^2)}=\frac{[q\mathsf{ch}(q)-\mathsf{sh}(q)]+[\mathsf{sh}(q)-q]\cos(t)}{q^3[\mathsf{ch}(q)-\cos(t)]} \tag{III.344}$$

for $q>0$, and in our case we know that $t=\frac{2\pi}{M}l, l\in\mathbb{Z}_M$. To prove this let us first check the degenerate case of $l=0$, which will cause the sum to collapse. Only the term $N=0$ will remain:

$$-2\sum_{N\in\mathbb{Z}}\frac{-1/2\cdot l^2+1/4!l^4+\dots}{(2\pi(N+l/M))^2(q^2+(2\pi)^2(N+l/M)^2)}\Big|_{l=0}=\frac{1}{q^2+(2\pi)^2\cdot 0}\cdot\sum_{N\in\mathbb{Z}}\delta(N+l/M,0)=\frac{1}{q^2} \tag{III.345}$$

on the other hand:

$$\frac{[q\mathsf{ch}(q)-\mathsf{sh}(q)]+[\mathsf{sh}(q)-q]\cos(0)}{q^3(\mathsf{ch}(q)-\cos(0))}=\frac{q\,\mathsf{ch}(q)-q}{q^3(\mathsf{ch}(q)-1)}=\frac{1}{q^2} \tag{III.346}$$

Hence, the claim is true for $t=0$. For $t\neq 0$, we invoke the following theorem due to Mittag-Leffler:

Theorem III.E.1. *(Mittag-Leffler) Let $a_1,a_2,\dots$ be a sequence with no finite convergence points and let P_k be polynomials without constant terms. Then there are functions meromorphic in the whole plane with poles precisely at a_k and corresponding singular part $P_k\left(\frac{1}{z-a_k}\right)$. In other words, the residual of n-th order in a_k is exactly the prefactor of the n-th power of P_k. The most general such meromorphic function may be written as*

$$f(z)=g(z)-\sum_{k=1}^{\infty}P_k\left(\frac{1}{z-a_k}\right)-h_k(z) \tag{III.347}$$

with g being entire, i.e. everywhere analytic, and h_k are suitably chosen polynomials, in such a way, that the convergence of the series is ensured.

Proof. The proof can be found in most standard books on complex analysis, e.g. [221].

It implies that any given meromorphic function $f(z)$ in $\mathbb{C}$ with poles a_k and corresponding principal parts of the unique Laurent expansion of $f(z)$ in a neighbourhood of a_k can be expanded in this series, where $g(z)$ is determined by $f(z)$.
We apply this theorem onto the function:

$$f(z):=\frac{\sqrt{z^2+q^2}\mathsf{ch}(\sqrt{z^2+q^2})-\mathsf{sh}(\sqrt{z^2+q^2})+[\mathsf{sh}(\sqrt{z^2+q^2})-\sqrt{z^2+q^2}]\cos(t)}{\sqrt{z^2+q^2}^3[\mathsf{ch}(\sqrt{z^2+q^2})-\cos(t)]} \tag{III.348}$$

which has poles in $a_N=\pm i\sqrt{q^2+(t+2\pi m)^2}$ of first order:

$$\mathrm{Res}_{a_m}\left(\frac{1}{\mathrm{ch}(\sqrt{x^2+q^2})-\cos(t)}\right)=\frac{1}{\pm i\sqrt{q^2+(t+2\pi N)^2}}\frac{t+2\pi N}{\sin(t)} \tag{III.349}$$

Thus the sum of the $P_k\left(\frac{1}{z-a_N}\right)$ becomes:

$$\begin{aligned}
&\sum_{N\in\mathbb{Z}}\frac{\mathsf{sh}(i(t+2\pi N))}{\sin(t)}\frac{\cos(t)-1}{i^3(t+2\pi N)^2}\times\\
&\qquad\times\left(\frac{1}{+i\sqrt{q^2+(t+2\pi N)^2}}\frac{1}{z-i\sqrt{q^2+(t+2\pi N)^2}}+\frac{1}{-i\sqrt{q^2+(t+2\pi N)^2}}\frac{1}{z+i\sqrt{q^2+(2\pi N)^2}}\right)\\
&=\sum_{N\in\mathbb{Z}}\frac{\cos(t)-1}{-i(t+2\pi N)^2\sqrt{q^2+(t+2\pi N)^2}}\left(\frac{1}{z-i\sqrt{q^2+(t+2\pi N)^2}}-\frac{1}{z+i\sqrt{q^2+(t+2\pi N)^2}}\right)\\
&=\sum_{N\in\mathbb{Z}}(-1/i)\frac{\cos(t)-1}{(t+2\pi N)^2\sqrt{q^2+(t+2\pi N)^2}}\left(\frac{z+i\sqrt{q^2+(t+2\pi N)^2}-z+i\sqrt{q^2+(2\pi N)^2}}{z^2+(q^2+(t+2\pi N)^2)}\right)\\
&=-2\sum_{N\in\mathbb{Z}}\frac{\cos(t)-1}{(t+2\pi N)^2(z^2+q^2+(t+2\pi N)^2)}
\end{aligned}$$

As this sum is already convergent for every z, we can neglect all the counter terms h_k and set them equal to zero when applying the Mittag-Leffler theorem. Consequently we know of the existence of an entire $g(z)$ such that:

$$f(z) = g(z) - 2 \sum_{N \in \mathbb{Z}} \frac{\cos(t) - 1}{(t + 2\pi N m)^2 (z^2 + q^2 + (t + 2\pi N)^2)} \tag{III.350}$$

Writing $z = x + iy$ it is easy to see, that the infinite sum tends to 0 locally uniformly in x as $y \to \pm\infty$. The same is true for $f(z)$ since it consists of four terms, each going either as $\sqrt{z^2 + c}^{-2}$ or $\sqrt{z^2 + c}^{-3}$. Thus, the same is true for $g(z)$ which is therefore bounded and entire, hence by Liouville's theorem constant. Since $g(iy) \to 0$ as $y \to +\infty$ the constant is zero. Lastly, we choose $z = 0$ and the claim (III.344) is shown!

We end up with

$$\begin{aligned} \hat{c}^*_M(k_0, l) =& \epsilon_M^2 \frac{[q_N \mathrm{ch}(q_N) - \mathrm{sh}(q_N)] + [\mathrm{sh}(q_N) - q_N] \cos(t_2)}{q_N^3 [\mathrm{ch}(q_N) - \cos(t_2)]} + \\ & - 2\epsilon_M^2 \sum_{N \in \mathbb{Z}} \frac{\cos(t_1) - 1}{(2\pi N + t_1)^2} \frac{1}{q_N^3} \frac{q_N \mathrm{ch}(q_N) - \mathrm{sh}(q_N) + (\mathrm{sh}(q_N) - q_N) \cos(t_2)}{\mathrm{ch}(q_N) - \cos(t_2)} \end{aligned} \tag{III.351}$$

The result has no manifest symmetry in $t_1 \leftrightarrow t_2$ but from the derivation it is clear that it must be. Note that each term in the sum remains finite for $\epsilon \to 0$ as the individual parts contribute inverse powers of ϵ_M: $(\cos(t) - 1)$ scales as $\mathcal{O}(\epsilon_M^2)$, since $t = k_R \epsilon_M l$ depends linearly on ϵ_M as well as $q = \epsilon_M^2 (p^2 + k_0)^2$. Thus $(q^2 + (t + 2\pi N)^2) = \mathcal{O}(\epsilon_M^2)$ if $N = 0$ or approaches a constant else.

III.E.2 Consistency check with the continuum covariance

The mere existence of a fixed point measure family described by the covariance (III.351) of the flow induced by (III.320) does not necessarily mean that it has any relation with the known continuum theory. We will thus invoke the consistency check also presented in the section *III.C. Example: Klein Gordon field I - Derivation*, which consists of looking at the cylindrical projection at resolution M of the continuum covariance $c := \frac{1}{2}\omega^{-1}$ in $D = 2$. The details are taken from [131]. Using that the covariance is given by (III.314), we find its projection to be

$$\begin{aligned} c_M(m, m') &= \epsilon_M^{-4} (I_M^\dagger \, c \, I_M)(m, m') = \\ &= \epsilon_M^{-4} \int_{m_1 \epsilon_M}^{(m_1+1)\epsilon_M} dx_1 \int_{m_2 \epsilon_M}^{(m_2+1)\epsilon_M} dx_2 \int_{m_1' \epsilon_M}^{(m_1'+1)\epsilon_M} dy_1 \int_{m_2' \epsilon_M}^{(m_2'+1)\epsilon_M} dy_2 \quad c(x, y) \end{aligned} \tag{III.352}$$

see [129] for more details. Using that the $e_n(x) := \frac{1}{R} e^{i k_R n \cdot x}$, $k_R = 2\pi/R$ define an orthonormal basis of $L_R = L_2([0, R)^2, d^2x)$ one finds the resolution of identity

$$\frac{1}{R^2} \sum_{n \in \mathbb{Z}^2} e^{i k_R (x - y) \cdot n} = \delta_R(x, y) := \delta_R(x_1, y_1) \delta_R(x_2, y_2) \tag{III.353}$$

We use this to write the covariance as

$$\begin{aligned} c(x, y) &= \frac{1}{2} \left(-\Delta_{Rx} + p^2\right)^{-1/2} \delta_R(x, y) = \int \frac{dk_0}{2\pi} \left(-\Delta_{Rx} + k_0^2 + p^2\right)^{-1} \delta_R(x, y) \\ &= \int \frac{dk_0}{2\pi} \sum_{n \in \mathbb{Z}^2} e_{nR}(y) \left(-\Delta_{Rx} + p^2 + k_0^2\right)^{-1} e_{nR}(x) = \frac{1}{R^2} \sum_{n \in \mathbb{Z}^2} e^{i k_R n \cdot (x - y)} \frac{1}{n^2 k_R^2 + k_0^2 + p^2} \end{aligned} \tag{III.354}$$

Now we can perform the integrals, e.g.

$$\int_{m_1 \epsilon_M}^{(m_1+1)\epsilon_M} dx_1 e^{i(2\pi) n_1 x_1} = \frac{1}{i k_R n_1} \left(e^{i k_R n_1 (m_1+1) \epsilon_M} - e^{i k_R n_1 m_1 \epsilon_M}\right) \tag{III.355}$$

where the case $n_1 = 0$ is obtained using de l'Hospital. We find with $k_M = 2\pi/M$

$$\begin{aligned} c_M(m, m') &= \epsilon_M^{-4} \frac{1}{R^2} \int \frac{dk_0}{2\pi} \sum_{n \in \mathbb{Z}^2} \frac{1}{n^2 k_R^2 + p^2 + k_0^2} \left(\int_{m_1 \epsilon_M}^{(m_1+1)\epsilon_M} dx_1 e^{i(2\pi) n_1 x_1}\right) \times \\ & \times \left(\int_{m_2 \epsilon_M}^{(m_2+1)\epsilon_M} dx_2 e^{i(2\pi) n_2 x_2}\right) \left(\int_{m_1' \epsilon_M}^{(m_1'+1)\epsilon_M} dy_1 e^{i(2\pi) n_1 y_1}\right) \left(\int_{m_2' \epsilon_M}^{(m_2'+1)\epsilon_M} dy_2 e^{i(2\pi) n_2 y_2}\right) \\ &= R^{-2} \int \frac{dk_0}{2\pi} \sum_{n \in \mathbb{Z}^2} \frac{1}{n^2 k_R^2 + p^2 + k_0^2} e^{i k_M n \cdot (m - m')} \frac{4}{k_M^4 n_1^2 n_2^2} [1 - \cos(k_M n_1)] \, [1 - \cos(k_M n_2)] \end{aligned} \tag{III.356}$$

We proceed exactly as earlier and thus split the sum over $n_j = l_j + MN_j$ with $l_j \in \mathbb{Z}_M$ and $N \in \mathbb{Z}^2$

$$c_M(m,m') = R^{-2}\epsilon_M^4 \int \frac{dk_0}{2\pi} \sum_{m\in\mathbb{Z}_M^2} e^{ik_M l\cdot(m-m')} \sum_{N\in\mathbb{Z}^2} \times \tag{III.357}$$
$$\times \frac{[1-\cos(k_M(l_1+MN_1)]\,[1-\cos(k_M(l_2+MN_2)]}{(l+MN)^2k_M^2+\epsilon_M^2(p^2+k_0^2)} \; \frac{4}{k_M^4(l_1+MN_1)^2(l_2+MN_2)^2}$$

from which we read off the Fourier transform of $c_M(m) = R^{-2}\sum_{l\in\mathbb{Z}_M^2} e^{k_M l\cdot m}\hat{c}_M(l)$

$$\hat{c}_M(k_0,l) = \epsilon_M^4 \sum_{N\in\mathbb{Z}^2} \times \tag{III.358}$$
$$\times \frac{[1-\cos(k_M(l_1+MN_1)]\,[1-\cos(k_M(l_2+MN_2)]}{(l+MN)^2k_M^2+q^2} \; \frac{4}{k_M^4(l_1+MN_1)^2(l_2+MN_2)^2}$$

Using the contour integral idea as in the previous subsection we obtain

$$\hat{c}_M(k_0,l) = -\frac{1}{2\pi i}\oint_\gamma dz \prod_{j=1,2} [\sum_{N_j\in\mathbb{Z}} \epsilon_M^2 \frac{1-\cos(k_M(l_j+MN_j))}{(l_j+MN_j)^2k_M^2+q_j(z)^2} \; \frac{2}{k_M^2(l_j+MN_j)^2}] \tag{III.359}$$

where $q_j(z)$ is the same as in the previous subsection. Now the two sums of the formula above are exactly the same that occurred in (III.134) with q^2 replaced by $q_j(z)^2$ and t replaced by $t_j = l_j k_M$. Thus, we can copy the result from there and find

$$\hat{c}_M(k_0,l) = -\frac{\epsilon_M^4}{2\pi i}\oint_\gamma dz \prod_{j=1,2} \frac{1}{q_j^3} \frac{q_j(z)\text{ch}(q_j) - \text{sh}(q_j) + [\text{sh}(q_j) - q_j]\cos(t_j)}{\text{ch}(q_j) - \cos(t_j)} \tag{III.360}$$

with $q_j \equiv q_j(z)$. Comparing (III.360) and (III.340) we see that both agree, thus the fixed point covariance family indeed coincides with the continuum covariance family.

III.E.3 Fixed points of the free scalar field for changed RG-flows

The aim of this section is to change the block-spin-transformation we have used so far and to check whether the fixed point is changed as well. For this, we quote from [131]. As has already been discussed in the third subsection of *III.D. Example: Klein Gordon field II - Properties* not every coarse graining map fulfils the cylindrical consistency relation which induces a corresponding relation on the family of coarse grained measures. Note that coincidence of continuum measures with their cylindrical (finite resolution) projections can only be deduced if one uses the same blocking kernel (which defines those projections). Thus, it a natural question to ask whether other maps of the kind $I_{M\to M'}$ apart from $M' = 2M$ will also lead to physically relevant theories. Due to the cylindrical consistency property of $I_{M\to M'}$ it is apparent that this is the case for all $M' = 2^n M$ for $n \in \mathbb{N}$. A natural extension would be to consider powers of any prime number. In this section we present how at least for the choice for $M' = 3M$ and $M' = 5M$ this indeed gives the same fixed point covariance and argue that it should be true for every choice of prime number. This would be useful because the set $\mathbb{N}$ is partially ordered and directed by $<$, but given $m_1, m_2 \in \mathbb{N}$ we do not always find $m_3 > m_1, m_2$ with $m_3 = m_1 2^{n_1} = m_2 2^{n_2}$.

If one considers $I_{M\to uM}$ with $u \in \mathbb{P}$ a prime number then the coarse graining map is given by

$$[I_{M\to uM} f_M](m) = f_M(\lfloor \frac{m}{u} \rfloor) \tag{III.361}$$

where $\lfloor . \rfloor$ is the component wise Gauss bracket. This map is easily checked to be cylindrically consistent, i.e. $I_{u^kM\to u^{k+l}M} \circ I_{M\to u^kM} = I_{M\to u^{k+l}M}$. To see this, we note that $\lfloor m/u^k \rfloor = m'$ if $m = m'u^k + r,\ r = 0,...u^k-1$ so that $\lfloor \lfloor m/u^l \rfloor / u^k \rfloor = m'$ for $\lfloor m/u^l \rfloor = m'u^k + r,\ k = 0,..,u^k-1$ that is for $m = (m'u^k + r)u^l + s,\ s = 0,..u^l-1$ i.e. $m = m'u^{k+l} + t,\ t = 0,..,u^{k+l}-1$ i.e. $m' = \lfloor m/u^{k+l} \rfloor$.

We now use these maps on our Gaussian example. For their covariances this implies

$$\begin{aligned}
\langle f_M, C_M^{(n+1)} f_M \rangle &= \epsilon_M^{2D} \sum_{m_1',m_2'\in\mathbb{Z}_M^D} f_M(m_1')f_M(m_2')C_M^{(n+1)}(m_1',m_2') \\
&= \langle I_{M\to uM} f_M, C_{uM}^{(n)} I_{M\to uM} f_M \rangle = \epsilon_{uM}^{2D} \sum_{m_1,m_2\in\mathbb{Z}_{uM}^D} f_M(\lfloor \frac{m_1}{u} \rfloor) f_M(\lfloor \frac{m_2}{u} \rfloor) C_{uM}^{(n)}(m_1,m_2) \\
&= \frac{\epsilon_{uM}^{2D}}{u^{2D}} \sum_{m_1',m_2'\in\mathbb{Z}_M^D} f_M(m_1')f_M(m_2') \sum_{\lfloor m_1/u \rfloor = m_1', \lfloor m_2/u \rfloor = m_2'} C_{uM}^{(n)}(m_1,m_2)
\end{aligned} \tag{III.362}$$

This allows to deduce by direct comparison:

$$C_M^{(n+1)}(m_1', m_2') = u^{-2D} \sum_{\delta', \delta'' \in \{0,1,..,u-1\}^D} C_{uM}^{(n)}(um_1' + \delta', um_2' + \delta'') \tag{III.363}$$

Again we employ translational invariance, i.e. $C_M^{(n)}(m_1, m_2) = C_M^{(n)}(m_1 - m_2)$ and find for the Fourier transform: ($k_M = \frac{2\pi}{M} = uk_{uM}$)

$$\begin{aligned} C_M^{(n+1)}(m_1', m_2') = &\sum_{l' \in \mathbb{Z}_M^D} e^{ik_M l'(m-m')} \hat{C}_M^{(n+1)}(l') \\ =& u^{-2D} \sum_{l \in \mathbb{Z}_{uM}^D} \hat{C}_{uM}^{(n)}(l) \sum_{\delta', \delta'' \in \{0,1,\dots,u-1\}^D} e^{ik_{uM} l \cdot (u(m_1'-m_2') + \delta' - \delta'')} \\ =& u^{-2D} \sum_{l' \in \mathbb{Z}_M^D} e^{ik_M l'(m_1'-m_2')} \sum_{\delta', \delta'', \delta \in \{0,1,\dots,u-1\}^D} \hat{C}_{3M}^{(n)}(l' + \delta M) e^{ik_{uM}(l'+\delta)\cdot(\delta'-\delta'')} \end{aligned} \tag{III.364}$$

whence

$$\hat{C}_M^{(n+1)}(l') = u^{-2D} \sum_{\delta \in \{0,1,\dots,u-1\}^D} \hat{C}_{uM}^{(n)}(l' + \delta M) \prod_{i=1}^{D} \frac{\sin(\frac{u}{2} k_{uM}(l_i' + \delta_i M))^2}{\sin(\frac{1}{2} k_{uM}(l_i' + \delta_i M))^2} \tag{III.365}$$

where we have used that the exponentials decouple, and that the geometric series can be performed explicitly

$$\sum_{\delta, \delta' \in \{0,\dots,u-1\}} e^{ia(\delta-\delta')} = \frac{1-e^{iau}}{1-e^{ia}} \frac{1-e^{-iau}}{1-e^{-ia}} = \frac{\sin(\frac{u}{2}a)^2}{\sin(\frac{1}{2}a)^2} \tag{III.366}$$

Since (III.365) states that the flow decouples in general and since we can write the initial covariance also in a decoupled form, this allows us to limit our further analysis to the $D = 1$ case without loss of generality.

The following explicit calculations are performed for the prime $u = 3$ as this illustrates what needs to be done also in the general case. The initial data of the RG-flow is given for $D = 1$ with $t = k_M l, q^2 = \epsilon_M^2(k_0^2 + p^2)$ by

$$\hat{c}_M^{(0)}(k_0, l) = \frac{\epsilon_M^2}{2(1-\cos(t)) + q^2} \tag{III.367}$$

In order to compute this flow, it is useful to recall the trigonometric addition theorems for the cosine function

$$\cos(x) + \cos(y) = 2\cos\left(\frac{x+y}{2}\right)\cos\left(\frac{x-y}{2}\right), \quad \cos(x)\cos(y) = \frac{1}{2}\left(\cos(x-y) + \cos(x+y)\right) \tag{III.368}$$

to note the following explicit values

$$\cos(\frac{1}{6}2\pi) = \frac{1}{2}, \qquad \cos(\frac{1}{3}2\pi) = -\frac{1}{2}, \qquad \cos(\frac{2}{3}2\pi) = -\frac{1}{2} \tag{III.369}$$

and to employ the *Chebyshev recursive method*, which states that for $N \in \mathbb{N}$:

$$\cos(Nx) = 2\cos(x)\cos((N-1)x) - \cos((N-2)x) \tag{III.370}$$

which is an easy expansion into exponentials and finds application in what follows for the case $N = 3$ and $x \to x/3$ to express $\cos(x) = 2\cos(x/3)\cos(2/3x) - \cos(x/3)$.

Equipped with these tools, we start to compute the RG flow of $I_{M\to 3M}$ by finding a common denominator of the sum in (III.365) assuming $\hat{c}^{(n)}$ could have been written in the form

$$\hat{c}_M^{(n)}(k_0, l) = \frac{\epsilon_M^2}{q^3} \frac{b_n(q) + c_n(q)\cos(t)}{a_n(q) - \cos(t)} \tag{III.371}$$

with suitably chosen functions a_n, b_n, c_n of q as we already know is true for (III.367). Then, the common denominator after one renormalisation step is generated by the linear combination of the of the three fractions in (III.365) and is given by:

$$\left[a_n(q) - \cos\left(\frac{t}{3}\right)\right]\left[a_n(q) - \left(\frac{t}{3} + M\frac{2\pi}{3M}\right)\right]\left[a_n(q) - \cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right)\right] =$$
$$= a_n(q)^3 - a_n(q)^2\left[\cos\left(\frac{t}{3}\right) + \cos\left(\frac{t}{3} + \frac{1}{3}2\pi\right) + \cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right)\right]_A$$
$$+ a_n(q)\left[\cos\left(\frac{t}{3}\right)\cos\left(\frac{t}{3} + \frac{1}{3}2\pi\right) + \cos\left(\frac{t}{3}\right)\cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right) + \cos\left(\frac{t}{3} + \frac{1}{3}2\pi\right)\cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right)\right]_B$$
$$- \left[\cos\left(\frac{t}{3}\right)\cos\left(\frac{t}{3} + \frac{1}{3}2\pi\right)\cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right)\right]_C$$

Each of the three prefactors in front of each power of $a_n(q)$ can now be evaluated precisely with the methods stated above. We obtain:

$$\left[\cos\left(\frac{t}{3}\right) + \cos\left(\frac{t}{3} + \frac{1}{3}2\pi\right) + \cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right)\right]_A = 0 \tag{III.372}$$

$$\left[\cos\left(\frac{t}{3}\right)\cos\left(\frac{t}{3} + \frac{1}{3}2\pi\right) + \cos\left(\frac{t}{3}\right)\cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right) + \cos\left(\frac{t}{3} + \frac{1}{3}2\pi\right)\cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right)\right]_B = -\frac{3}{4} \tag{III.373}$$

$$\left[\cos\left(\frac{t}{3}\right)\cos\left(\frac{t}{3} + \frac{1}{3}2\pi\right)\cos\left(\frac{t}{3} + \frac{2}{3}2\pi\right)\right]_C = \frac{1}{4}\cos(t) \tag{III.374}$$

So we get for the denominator

$$\frac{1}{4}\left(\left[4a_n(q)^3 - 3a_n(q)\right] - \cos(t)\right) \tag{III.375}$$

which is again of the form that (III.371) had. Moreover, we note that the t-independent part of (III.375) is exactly the right hand side of the triple-angle formula for cos, cosh:

$$a(3q) = 4a(q)^3 - 3a(q) \tag{III.376}$$

hence with the choice of $a(q) = \mathsf{ch}(q)$ we have found a fixed point for the flow induced onto the $a_n(q)$.
For the numerator, we continue in the same manner. After some pages of calculation, one finds it to be given by

$$(3 + 4\cos(t/3) + 2\cos(2/3t))(b_n - c_n \cdot \cos(t/3))(a_n - \cos(t/3 + 2\pi/3))\times$$
$$\times (a_n - \cos(t/3 + 2/3 \cdot 2\pi))(3 + 4\cos(t/3 + 2\pi/3) + 2\cos(2t/3 + 2/3 \cdot 2\pi))(a_n - \cos(t/3))\times$$
$$\times (a_n - \cos(t/3))(a_n - \cos(t/3 + 2/3 \cdot 2\pi))(3 + 4\cos(t/3 + 2/3 \cdot 2\pi) + 2\cos(2/3t + 4/3 \cdot 2\pi))\times$$
$$\times (b_n - c_n \cdot \cos(t/3 + 2/3 \cdot 2\pi))(a_n - \cos(t/3 + 2\pi/3)(b_n - c_n \cdot \cos(t/3 + 2\pi/3)))$$
$$= \ldots = \left(-\frac{3}{4} + 6a_n + 9a_n^2\right)b_n - 6a_n(1 + a_n)c_n + \frac{3}{4}\left(4(1 + a_n)b_n - (3 + 4a_n + 4a_n^2)c_n\right)\cos(t) \tag{III.377}$$

Thus, also the numerator is cast again into an expression of the form $b_{n+1} + c_{n+1}\cos(t)$. We can already make use of the fact, that at the fixed point one has $a = \cosh(q)$. Making an educated guess and trying whether

$$b = q\mathsf{ch}(q) - \mathsf{sh}(q), \qquad c = \mathsf{sh}(q) - q \tag{III.378}$$

are solutions of the fixed point equation determined by (III.377) one uses the triple-angle formula for the sine function

$$\sin(3x) = 2\cos(x)\sin(2x) - \sin(x) = -2\cos(2x)\sin(x) - \sin(x) \tag{III.379}$$

and obtains indeed by plugging (III.378) into (III.377):

$$3(1 + \cosh(q))(q\mathsf{ch}(q)) - \frac{1}{4}(3 + 4\mathsf{ch}(q) + 4\mathsf{ch}(q)^2)(-\mathsf{sh}(q) + q) = \frac{3}{4}\left[-3q + \mathsf{sh}(3q)\right] \tag{III.380}$$

and

$$\left(-\frac{3}{4} + 6\mathsf{ch}(q) + 9\mathsf{ch}(q)^2\right)(\mathsf{ch}(q) - \mathsf{sh}(q)) - 6\mathsf{ch}(q)(1 + \mathsf{ch}(q))(-\mathsf{sh}(q) + q) = \frac{3}{4}\left[3q\mathsf{ch}(3q) - \mathsf{sh}(3q)\right] \tag{III.381}$$

which presents indeed the triple angle formula, up to the common prefactor of $3/4$. The factor $1/4$ gets cancelled by the pre factor of $1/4$ in front of a_n in (III.375). The factor 3 cancels against a factor 3^{-1} which is obtained as follows: the map itself was defined with a prefactor 3^{-2}, the factor q^{-3} gives 3^3 and the ϵ_M^2 gives 3^{-2} which altogether gives a factor 3^{-1}. Hence we have indeed found exactly the same fixed point under the under $M \to 3M$ coarse graining map as we found for the $M \to 2M$ coarse graining map!

We did the same calculations also for the prime $u = 5$ which is considerably more work, but all steps are literally the same and also the fixed point is the same. For reasons of space, we do not display these calculations here and leave it to the interested reader as an exercise. For the general prime we do not have a proof available yet but hope to be able to supply it in a future publication. However, we do not expect any changes. In any case, for whatever primes the fixed point stays the same (it holds at least for $u = 2, 3, 5$) the statement is also true for all dimensions due to the factorising property. This factorising property also makes it possible to study in higher dimensions more complicated hypercuboid like coarse graining block transformations rather than hypercube like ones. In order to illustrate this, we give some details for the case $D = 2$ dimensions of a rectangle blocking with $u_1 = 2$ for the first direction and $u_2 = 3$ for the second. The map is consequently $I_{(M_1,M_2)\to(2M_1,3M_2)} = I_{M_1\to 2M_1} \times I_{M_2\to 3M_2}$. The naively discretised Laplacian on a lattice with different spacings $\epsilon_{M_1}, \epsilon_{M_2}$ is given as (here: $2\epsilon_{M_1} = 3\epsilon_{M_2}$)

$$\begin{aligned}(\Delta_M f_M)(m) &:= \\ &= \frac{1}{\epsilon_{M_1}^2}\left(f_M(m+e_1) + f_M(m-e_1) - 2f_M(m)\right) + \frac{1}{\epsilon_{M_2}^2}\left(f_M(m+e_2) + f_M(m-e_2) - 2f_M(m)\right)\end{aligned} \tag{III.382}$$

Hence the same strategy from (III.328) works again and gives us:

$$\begin{aligned}\hat{C}_M^{(0)}(k_0, l) &= \left(-\frac{1}{\epsilon_{M_1}^2}(2\cos(k_{M_1}l_1) - 2) - \frac{1}{\epsilon_{M_2}^2}(2\cos(k_{M_2}l_2) - 2) + p^2 + k_0^2\right)^{-1} \\ &= \frac{1}{2\pi i}\oint_\gamma dz \frac{1}{z + (k_0^2+p^2)/2 - \frac{2}{\epsilon_{M_1}^2} - \frac{2}{\epsilon_{M_1}^2}\cos(k_{M_1}l_1)} \; \frac{1}{z - (k_0^2+p^2)/2 + \frac{2}{\epsilon_{M_2}^2} + \frac{2}{\epsilon_{M_2}^2}\cos(k_{M_2}l_2)} \\ &= -\frac{1}{2^3\pi i}\oint dz \frac{\epsilon_{M_1}^2}{\epsilon_{M_1}^2(z + k_0^2 + p^2/2)/2 + 1 - \cos(k_{M_1}l_1)} \; \frac{-\epsilon_{M_2}^2}{\epsilon_{M_2}^2(-z + k_0^2 + p^2/2)/2 + 1 - \cos(k_{M_2}l_2)}\end{aligned} \tag{III.383}$$

So both directions decouple and yield, as already shown the same fixed point! It remains to compute the integral which is exactly the same as (III.340).

A further immediate consequence is that at this fixed point, one could also consider the flow of arbitrary concatenations of different coarse-graining maps, independently for each direction, e.g. ...$I_{6M\to 12M} I_{2M\to 6M}$ $I_{M\to 2M}$... and we see that all of them have the same fixed point. We conclude that the fixed point is quite robust under rather drastic changes of the coarse graining map.

III.E.4 Rotational Invariance of the lattice fixed point theory

We now turn our attention towards the much discussed question of *rotational invariance* [114, 212, 213, 222–225]. By this we mean that most Hamiltonians for continuum theories on Minkowski space have $SO(D)$ as a symmetry group besides spatial translation invariance. On the one hand, a fixed lattice certainly breaks rotational invariance and in the case of a hypercubic lattice reduces the invariance to rotations by multiples of $\pm\pi/2$ around the coordinate axes. On the other hand, it is clear that the cylindrical projections of a rotationally invariant measure in the continuum with respect to smearing functions adapted to the family of hypercubic lattices in question must carry an imprint of that continuum rotation invariance. In other words, there must exist a criterion at finite lattice resolution, whether the corresponding lattice measure qualifies as the cylindrical projection of a continuum rotationally invariant measure.

In this section we identify such a notion of *rotational invariance* at finite resolution at least for the case of scalar field theories. This has been done first in [131]. We then successfully test this criterion for the fixed point covariance $\hat{c}_M^*(k_0, l = (l_1, l_2))$ in $D = 2$ for the free Klein Gordon field. Due to the factorisation property and due to the possibility of presenting any rotation in terms a composition of rotations about the coordinate axes, we can reduce our attention to two spatial dimensions. For this purpose, we will adopt the strategy from *III.D.5. Perfect Lattice Laplacian* and smear the covariance with some time-independent test functions $f(s, r) = f_M(r), f'(s', r')f'_M(r')$ to obtain $\delta_{k_0,0}$. Hence, in the remainder of this section, we suppress the label k_0 for most of the time.

We follow closely the calculations from [131]. This presents an example for how the Hamiltonian renormalisation scheme is able to detect the restoration of continuum properties of the classical theory which upon naive regularisation were lost in the quantisation process.

The lattice rotational invariance condition

Given the IR-restricted compact submanifold of σ, i.e. the D-dimensional torus σ_R with periodic boundary conditions and length R, one must be precise what one means by rotations. In order to rotate the system around $x_0 \in \sigma_R$ one uses the Euclidian metric on the torus to identify all points as a set S_r which have distance $r > 0$ to the central point x_0. We then choose S_r in order to construct a representation of $\mathsf{SO}(D)$ on it, e.g. in $D = 2$ one has $\Pi : \mathsf{SO}(2) \mapsto \mathsf{GL}(\sigma_R)$ with $\Pi(2\pi) = \mathrm{id}$ and $\Pi(\alpha)\Pi(\beta) = \Pi(\alpha + \beta)$, where we label the elements of the one-dimensional $SO(2)$ by $\alpha, \beta \in [0, 2\pi)$. Without loss of generality we will consider in the following $x_0 = 0$. Indeed, upon considering a chart in Cartesian coordinates that includes some complete S_r with $r < R/2$ this means we can write the action of a rotation on one of those S_r as a matrix ($x \in S_r$)

$$\Pi(\alpha) \cdot x = \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{pmatrix} \cdot x \tag{III.384}$$

Note that the rotations for $S_{r \geq R/2}$ are not described by a linear transformation due to the non-trivial boundary conditions. However, any $r < R/2$ will serve our purposes.

In the remainder of this section we limit the analysis to $D = 2$ as, once rotational invariance is established for all rotations in an arbitrary plane, any other rotation can be understood as multiple rotations in suitable planes. Further we employ the ideas of [212, 213]: instead of considering arbitrary angles in $[0, 2\pi)$, it suffices to show invariance under rotations of only one angle θ given that $\theta/(2\pi)$ is irrational. This is because the sequence

$$\mathbb{N} \to [0, 2\pi);\ n \mapsto \theta_n := n \cdot \theta \mod 2\pi \tag{III.385}$$

lies dense in $[0, 2\pi)$, i.e. $\forall \theta' \in [0, 2\pi)$ there exists a partial sequence $j \mapsto \theta_{n_j} \to \theta'$. Hence we can define the rotation by the angle θ' as

$$\Pi(\theta') := \lim_{\theta_{n_j} \to \theta'} \Pi(\theta)^{n_j} \tag{III.386}$$

It follows, assuming suitable continuity properties, that invariance under all these angles would be established, once it is shown for θ. In this paper we specialise to the angle θ defined by $\cos(\theta) = 3/5, \sin(\theta) = 4/5$ as it is indeed irrational. A proof for this and further properties can be found in [213].

By the above considerations we can give meaning to the term *rotational invariance* as a condition on the continuum Hilbert space measure ν. It is called rotationally invariant provided that for any measurable function g we have $\nu(g) = \nu(r(\theta)^* \cdot g)$ where $(r(\theta)^* \cdot g)[\phi] = g[r(\theta) \cdot \phi]$ and $[r(\theta) \cdot \phi](x) = \phi(\Pi(-\theta) \cdot x)$. Since ν is defined by its generating functional, we may restrict to the functions $g = w[f]$ for which in case of a scalar theory $r(\theta)^* w[f] = w[r(-\theta) \cdot f]$. We now translate this into a condition on the cylindrical projections ν_M of ν defined by $\nu_M(w_M[f_M]) := \nu(w[I_M f_M])$ where

$$(I_M f_M)(x) := \sum_{m \in \mathbb{Z}_M^2} f_M(m) \chi_{m\epsilon_M}(x),\ \chi_{m\epsilon_M}(x) = \prod_{a=1,2} \chi_{[m^a \epsilon_M, (m^a+1)\epsilon_M)}(x^a) \tag{III.387}$$

It follows that $r(-\theta) \cdot I_M f_m$ cannot be written as linear combinations of functions of the form $I_M f'_M$ because $r(-\theta) \cdot \chi_{M\epsilon_M}$ is the characteristic function of the rotated block. Hence the rotational invariance of ν does not have a direct translation into a condition of the ν_M. While we can define a new embedding map by

$$I_{\theta M} : L_M \to L \tag{III.388}$$

$$f_M \mapsto [I_{\theta M} f_M](x) := \sum_{m \in \mathbb{Z}_M^2} f_M(m) \chi_{m\epsilon_M}(\Pi(\theta) \cdot x) \tag{III.389}$$

the renormalisation flow defined by it may result in a fixed point covariance family $c^*_{\theta M}$ different from c^*_M. It is therefore a non-trivial question to ask what one actually means by *rotational invariance of a discrete lattice theory* or more precisely of a family of corresponding measures.

The idea is to consider both families (i.e. the unrotated theory described by the covariances c^*_M and the rotated one described by the covariances $c^*_{\theta M}$) as coarse-grained versions of *common* finer lattices with spacing ϵ_{5M} which is why we chose the above particular angle θ. The rotation of the coarse, unrotated lattice is a sublattice of the fine unrotated lattice called *discrete rotation* and is defined by

$$D_\theta : \mathbb{Z}_M^2 \to \mathbb{Z}_{5M}^2;\ m \mapsto \Pi(\theta) \cdot m \tag{III.390}$$

This map can be extended to

$$D_\theta \mathbb{Z}^2_{5M} \to \mathbb{Z}^2_{5M} m \mapsto \lfloor \Pi(\theta) \cdot m \rfloor \tag{III.391}$$

which maps the whole rotated finer lattice into the unrotated finer lattice.

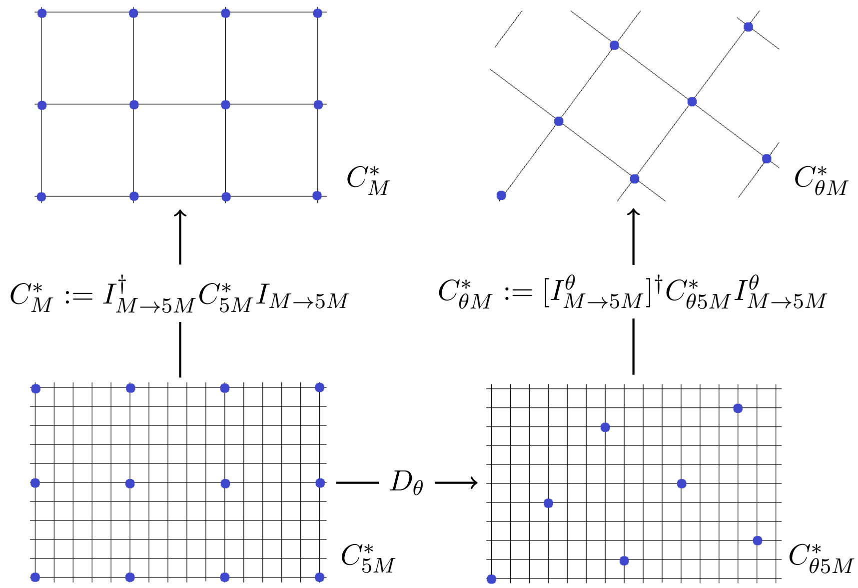

Abbildung III.7: Fixed point covariances C^*_M, $C^*_{\theta M}$ on lattices rotated relative to each other by the irrational angle θ (such that $\cos(\theta) = 3/5$) can be related by a common refined unrotated lattice and a map D_θ, called discrete rotation.

The condition that we are about to derive holds for general measures, but we also note in tandem the corresponding specialisation to Gaussian ones for a later test on our model free theory. Suppose then that ν^* is a rotationally invariant (Gaussian) measure, that is, for its generating functional (covariance) we have

$$\nu^*(w[f]) = \nu^*(w[\Pi(\theta) \cdot f]) \;\; (c^* = \Pi(\theta)^\dagger c^* \Pi(\theta)) \tag{III.392}$$

This means that for the cylindrical projections we have the identity

$$\nu^*_M(w_M[f_M]) = \nu^*(w[I_M f_M]) = \nu^*(w[\Pi(\theta) I_M f_M]) \;\; (c^*_M = [\Pi(\theta) I_M]^\dagger c^* [\Pi(\theta) I_M]) \tag{III.393}$$

Now

$$(\Pi(\theta) I_M f_M)(x) = \sum_{m \in \mathbb{Z}^2_M} f_M(m) \chi_{m,\epsilon_M}(\Pi(\theta)^{-1} \cdot x) \tag{III.394}$$

Let $B_{m,M}$ be the square (block) of which χ_{m,ϵ_M} is the characteristic function. Then

$$(\Pi(\theta) \cdot \chi_{m,\epsilon_M})(x) = \chi_{m,\epsilon_M}(\Pi(\theta)^{-1} \cdot x) = \chi_{\Pi(\theta) \cdot B_{m,M}}(x) \tag{III.395}$$

is the characteristic function of the rotated block of the coarse lattice with base (lower left corner) now at $\Pi(\theta) \cdot m \in \mathbb{Z}^2_{5M}$. Since we have the disjoint decomposition

$$B_{m,M} = \cup_{m' \in \mathbb{Z}^2_{5M} \cap B_{m,M}} B_{m',5M} \tag{III.396}$$

we have

$$\Pi(\theta) B_{m,M} = \sum_{m' \in \mathbb{Z}^2_{5M} \cap B_{m,M}} \Pi(\theta) B_{m',5M} \approx \sum_{m' \in \mathbb{Z}^2_{5M} \cap B_{m,M}} B_{D_\theta \cdot m',5M} \tag{III.397}$$

where we have replaced in the last step the rotated blocks of the fine lattice, which before rotation compose the unrotated block of the coarse lattice, by those unrotated blocks of the fine lattice with the bases at the points defined by D_θ. This is an approximation only, but it is better than one might think because the difference between the two functions only affects those blocks $B_{D_\theta \cdot m',5M}$ which intersect the boundary of $B_{\Pi(\theta) \cdot m,M}$. We will come back to the quality of this approximation below.

In any case, the last line in (III.397) defines an embedding $I^\theta_{M\to 5M}:\ L_M \to L_{5M}$ by

$$(I^\theta_{M\to 5M} f_M)(m') = \sum_{m''\in\mathbb{Z}^2_{5M}} \delta_{m',D_\theta\cdot m''} \sum_{m\in\mathbb{Z}^2_M} \delta_{m''\in B_{m,M}}\, f_M(m) \tag{III.398}$$

such that $I_{5M}\circ I^\theta_{M\to 5M}$ approximates $\Pi(\theta)\cdot I_M$ in the sense specified below. Thus

$$\nu^*_M(w_M[f_M]) \approx \nu^*(w[I_{5M} I^\theta_{M\to 5M} f_M]) = \nu^*_{5M}(w_{5M}[I^\theta_{M\to 5M} f_M]) \tag{III.399}$$

or for the Gaussian case

$$c^*_M \approx [(I_{5M}\circ I^\theta_{M\to 5M}]^\dagger c^* [I_{5M}\circ I^\theta_{M\to 5M}] = [I^\theta_{M\to 5M}]^\dagger c^*_{5M} I^\theta_{M\to 5M} \tag{III.400}$$

To write this just in terms of a single measure (covariance), we use cylindrical consistency $\nu^*_M(w_M[f_M]) = \nu^*_{5M}(w_{5M}[I_{M\to 5M} f_M])$ or $c^*_N = I^\dagger_{M\to 5M} c^*_{5M} I_{M\to 5M}$ to find

$$\nu^*_{5M}(w_{5M}[I^\theta_{M\to 5M} f_M]) \approx \nu^*_{5M}(w_{5M}[I_{M\to 5M} f_M]) \tag{III.401}$$

or

$$I^\dagger_{M\to 5M} c^*_{5M} I_{M\to 5M} \approx (I^\theta_{M\to 5M})^\dagger c^*_{5M} I_{M\to 5M} \tag{III.402}$$

as a lattice version for rotational invariance for (Gaussian) measures for scalar field theories.

To specify the quality of the approximation depends on the details and properties of the corresponding measure family. The following result is targeted to the class of Gaussian measures.

Lemma III.E.1. *Suppose that c^* is the covariance of a rotationally invariant Gaussian measure whose kernel is differentiable in the sense of distributions. Then*

$$\{c^*_M - [I^\theta_{M\to 5M}]^\dagger c^*_{5M} I^\theta_{M\to 5M}\}(m_1,m_2) = O(\epsilon^5_M) \tag{III.403}$$

for all $m_1, m_2 \in \mathbb{Z}^2_M$. The coefficient of ϵ^5_M is independent of M. Note that $c^*_M(m_1,m_2) = O(\epsilon^4_M)$ in $D=2$.

Beweis. Let $B^\theta_{m,M} = \cup_{m'\in\mathbb{Z}^2_{5M}\cap B_{m,M}} B_{D_\theta m',5M}$ and $S^\theta_{m,M} := \Pi(\theta)B_{m,M}\cap B^\theta_{m,M}$. Denote $\Delta^{\theta+}_{m,M} = \Pi(\theta)B_{m,M} - S^\theta_{m,M}$ and $\Delta^{\theta-}_{m,M} = B^\theta_{m,M} - S^\theta_{m,M}$. The sets $\Delta^{\theta\pm}_{m,M}$ are homeomorphic since $B^\theta_{m,M}$ consists of the squares of $\mathbb{Z}^2_{5M}$ whose lower left corner lies in $\Pi(\theta)B_{m,M}$. Thus $B^\theta_{m,M}$ lacks parts of $\Pi(\theta)B_{m,M}$ at the left two boundaries of $\Pi(\theta)B_{m,M}$ while $B^\theta_{m,M}$ exceeds $\Pi(\theta)B_{m,M}$ at its two right boundaries. Hence $\Delta^{\theta\pm}_{m,M}$ are complementary disjoint sets whose joint measure is equal to the measure of an integer number of squares of the lattice $\mathbb{Z}^2_{5M}$. They also have the same Lebesgue measure because $\Pi(\theta)B_{m,M}$ has measure ϵ^2_M due to rotational invariance of the Lebesgue measure and $B^\theta_{m,M}$ has measure $5^2\epsilon^2_{5M} = \epsilon^2_M$ because D_θ is injective as is easy to check so that $B^\theta_{m,M}$ consists of 25 squares of the lattice $\mathbb{Z}^2_{5M}$. Let $h: \Delta^{\theta+}_{m,M} \mapsto \Delta^{\theta-}_{m,M}$ be the corresponding homeomorphism which can be written in the form $h(x) = x + g(x)\epsilon_M$ with $||g(x)|| \le \sqrt{2}$ as the maximal distance between points in the two sets is $\sqrt{2}\epsilon_M$. Then by rotational invariance we obtain the third line in:

$$\begin{aligned}
& \{c^*_M - [I^\theta_{M\to 5M}]^\dagger c^*_{5M} I^\theta_{M\to 5M}\}(m_1,m_2) = \\
= \;& \{\int_{B_{m_1,M}} d^2x \int_{B_{m_2,M}} d^2y - \int_{B^\theta_{m_1,M}} d^2x \int_{B^\theta_{m_2,M}} d^2y\} c(x,y) \\
= \;& \{\int_{\Pi(\theta)B_{m_1,M}} d^2x \int_{\Pi(\theta)B_{m_2,M}} d^2y - \int_{B^\theta_{m_1,M}} d^2x \int_{B^\theta_{m_2,M}} d^2y\} c(x,y) \\
= \;& \{\int_{S^\theta_{m_1,M}} d^2x \int_{\Delta^{\theta+}_{m_2,M}} d^2y + \int_{\Delta^{\theta+}_{m_1,M}} d^2x \int_{S^\theta_{m_2,M}} d^2y + \int_{\Delta^{\theta+}_{m_1,M}} d^2x \int_{\Delta^{\theta+}_{m_2,M}} d^2y \\
& - \int_{S^\theta_{m_1,M}} d^2x \int_{\Delta^{\theta-}_{m_2,M}} d^2y - \int_{\Delta^{\theta-}_{m_1,M}} d^2x \int_{S^\theta_{m_2,M}} d^2y - \int_{\Delta^{\theta-}_{m_1,M}} d^2x \int_{\Delta^{\theta-}_{m_2,M}} d^2y\} c(x,y) \\
= \;& \int_{S^\theta_{m_1,M}} d^2x \int_{\Delta^{\theta+}_{m_2,M}} d^2y [c(x,y) - c(x, y+g(y)\epsilon_M)] + \int_{\Delta^{\theta+}_{m_1,M}} d^2x \int_{S^\theta_{m_2,M}} d^2y [c(x,y) - c(x+g(x)\epsilon_M, y)] \\
& + \int_{\Delta^{\theta+}_{m_1,M}} d^2x \int_{\Delta^{\theta+}_{m_2,M}} d^2y [c(x,y) - c(x+g(y)\epsilon_M, y+g(y)\epsilon_M]
\end{aligned} \tag{III.404}$$

from which the claim now follows by considering a power series expansion of c.

□

The lemma does not tell us anything about the size of the coefficient of ϵ_M^5 and thus of the actual quality at given M, however, assuming that the coefficient is finite, for sufficiently large M the approximation error is as small as we want compared to the value of the discrete kernel $c_M^*(m_1, m_2)$.

We translate the approximant $c_{M\theta}^* := [I_{M\to 5M}^\theta]^\dagger c_{5M}^* I_{M\to 5M}^\theta$ whose coefficients are explicitly given by (using translation invariance and (III.398))

$$c_{M\theta}^*(m) = \frac{1}{5^4} \sum_{\delta_1,\delta_2\in\{0,...,4\}^2} c_{5M}^*(D_\theta(5m + (\delta_1 - \delta_2))) \tag{III.405}$$

into the corresponding Fourier coefficients over which we have better analytic control

$$\begin{aligned} c_{\theta M}^*(m) &= \sum_{l\in\mathbb{Z}_M^2} e^{ik_M l\cdot m} \hat{c}_{\theta M}^*(l) \qquad\qquad \text{(III.406)} \\ &= \frac{1}{5^4} \sum_{l'\in\mathbb{Z}_{5M}^2} \sum_{\delta_1,\delta_2\in\{0,...,4\}^2} e^{ik_{5M} l'\cdot D_\theta(5m+(\delta_1-\delta_2))} \hat{c}_{5M}^*(l') = \\ &= \frac{1}{5^4} \sum_{l'\in\mathbb{Z}_{5M}^2} \sum_{\delta_1,\delta_2\in\{0,...4\}^2} e^{ik_{5M}(D_\theta^{-1} l')\cdot(5m+\delta_1-\delta_2)} \hat{c}_{5M}^*(l') = \\ &= \frac{1}{5^4} \sum_{l\in\mathbb{Z}_M^2} \sum_{\delta\in\{-2,...,2\}^2} e^{ik_M l\cdot m} e^{ik_M M\delta\cdot m} \sum_{\delta_1,\delta_2\in\{0...4\}^D} e^{ik_{5M}(l+M\delta)\cdot(\delta_1-\delta_2)} \hat{c}_{5M}^*(D_\theta(l+M\delta)) \end{aligned}$$

where we used the fact that D_θ is a bijective map to obtain the third line, as well as for the fourth line, where we have relabelled $D_\theta l' \to l'$ and split $l' = l + M\delta$. We have chosen the interval $\delta \in \{-2, ..., 2\}^2$ because of its symmetry regarding rotations around the point $x_0 = 0$, which are considered here, using the periodicity of the boundary conditions. Performing the sum over δ_1, δ_2 and comparing coefficients we obtain

$$\hat{c}_{\theta M}^*(l) = \frac{1}{5^4} \sum_{\delta\in\{-2...2\}^2} \prod_{i=1}^2 \frac{\sin(\frac{5k_{5M}}{2}[l_i + M\delta_i])^2}{\sin(\frac{k_{5M}}{2}[l_i + M\delta_i])^2} \hat{c}_{5M}^*(D_\theta(l + M\delta)) \tag{III.407}$$

which can now be readily numerically compared to $c_M^*(l)$ (after writing it as an integral over k_0).

We remark that for rotational invariance under an arbitrary angle θ' we pick an approximant $n \cdot \theta$ mod 2π for sufficiently large $n \in \mathbb{N}$. Then, the whole analysis can be repeated using the $M \to 5^n M$ refinement since $\Pi(\theta)^n$ is a matrix with rational entries with common denominator 5^n. Since the sets $\Delta_{m,5^n}^{\theta\pm}$ involve an order of 4×5^n boundary squares of respective measure $\epsilon_{5^n M}^2 = \epsilon_M^2 5^{-2n}$ the relative error here would even be smaller, i.e. of order $5^{-n}\epsilon_M$.

III.E.5 Numerical investigation for rotational invariance

In this subsection, we test our criterion numerically using the fixed point theory in $D = 2$, which we know to be rotationally invariant in the continuum. We do not perform this numerical investigations anew, but cite the work from [131].

First, we verify that the family of covariances c_M^* is invariant under rotations by $\pm\pi/2$. It suffices to consider the rotation $\Pi(\pi/2)$ and apply this to (III.340) which is symmetric under exchange of $t_1 \leftrightarrow t_2$ (since we could have interchanged the roles of those in the contour integral). We have

$$\begin{aligned} &\langle r(\pi/2) f_M, c_M^* r(\pi/2) f_M' \rangle_M = \\ &= \epsilon_M^4 \sum_{m,m'\in\mathbb{Z}_M^2} f_M(\Pi(\pi/2)\cdot m) f_M'(\Pi(\pi/2)\cdot m') \sum_{n\in\mathbb{Z}_M^2} e^{ik_M n\cdot(m_1-m_2)} \hat{c}_M^*(n_1, n_2) \\ &= \epsilon_M^4 \sum_{m,m'\in\mathbb{Z}_M^2} f_M(m) f_M'(m') \sum_{n\in\mathbb{Z}_M^2} e^{ik_M n\cdot\Pi(\pi/2)^{-1}(m-m')} \hat{c}_M^*(n_1, n_2) \\ &= \epsilon_M^4 \sum_{m,m'\in\mathbb{Z}_M^2} f_M(m) f_M'(m') \sum_{n\in\mathbb{Z}_M^2} e^{ik_M n\cdot(m-m')} \hat{c}_M^*((\Pi(\pi/2)^{-1}\cdot n)_1, (\Pi(\pi/2)^{-1}\cdot n)_2) \qquad \text{(III.408)} \end{aligned}$$

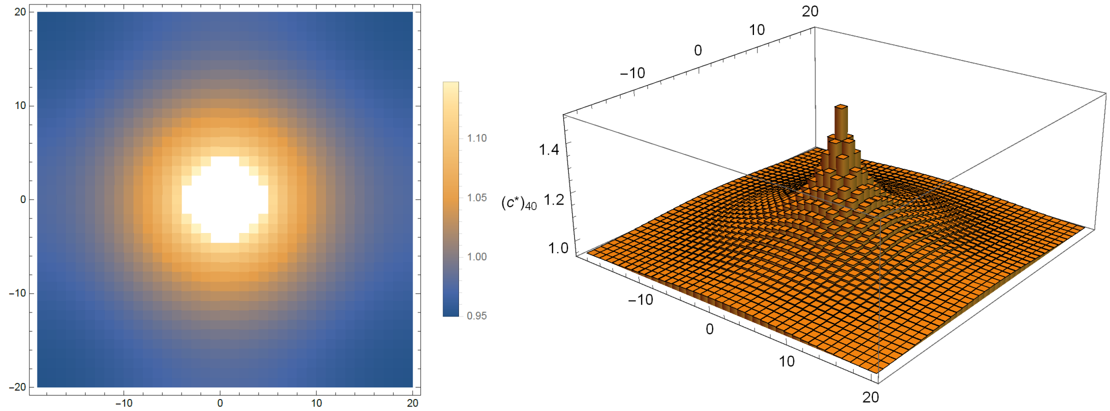

Abbildung III.8: The covariance $c^*_M(m)$ of the fixed point theory in $D = 2$ spatial dimensions. We have chosen the IR cut-off $R = 1$, mass $p = 1$, and $k_0 = 0$. The torus $[0, 1)^2$ is approximated by a lattice with $M = 40$ points in each direction, where the point $m = (0, 0)$ lies in the centre of the plotted grid. As one can see, the contributions from next neighbour frequencies are highly suppressed.

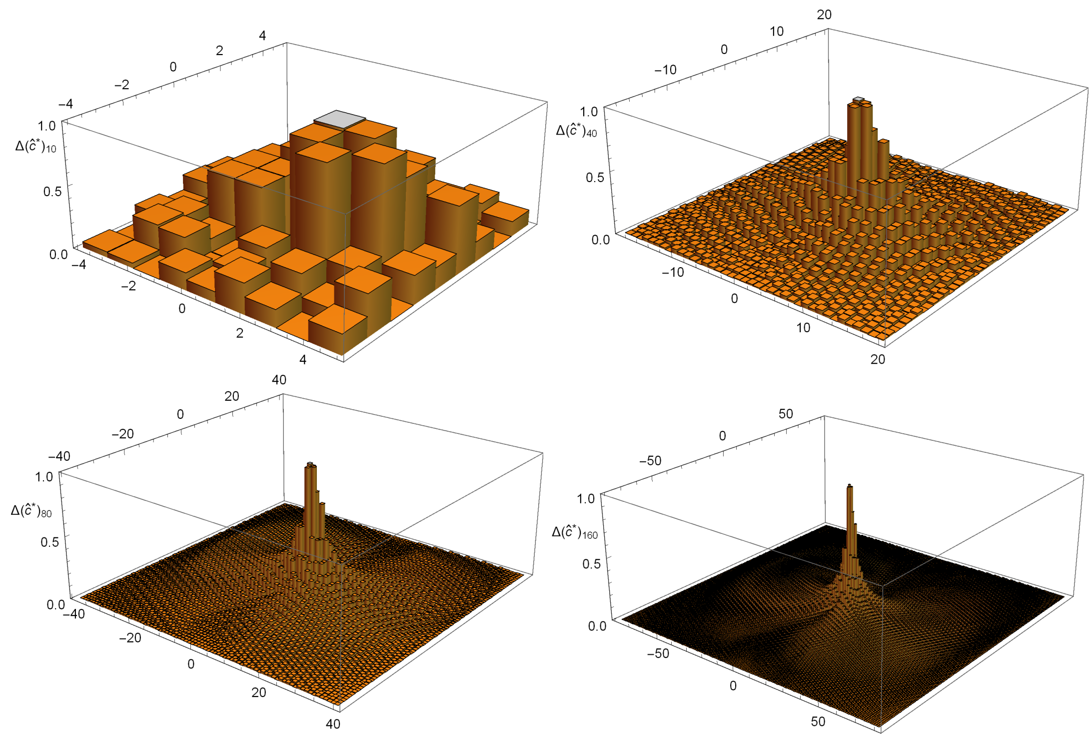

Abbildung III.9: For lattices of size $M = 10,\ 40,\ 80,\ 160$ the relative deviation $\Delta\hat{c}^*_M(l) = [|\hat{c}^*_M - \hat{c}^*_{\theta,M}|/\hat{c}^*_M](k_0 = 0, l)$ is plotted for $l \in \mathbb{Z}^2_M$ with mass $p = 1$ and IR cut-off $R = 1$. High values of $\Delta\hat{c}^*_M$ indicate non-invariance of the covariance at given resolution under rotations. (The *grey* data point lies outside the plotted range of $[0, 1)$, with numerical value ≈ 40.) We find that the relative deviation is non-vanishing everywhere at finite resolution, however it decreases with M^{-1} because $\hat{c}^*_M - \hat{c}^*_{\theta M} \sim O(\epsilon^5_M) \sim \hat{c}^*_M\epsilon_M$. This is the approximative behaviour of a rotationally invariant fixed point theory. For $M = 160$ the computed covariance features already rotational invariance to a high precision.

Thus, for $\pi/2$ equation (III.403) becomes the condition:

$$\hat{c}^*_M(n_1, n_2) = \hat{c}^*_M(-n_2, n_1)\ , \quad \forall n = (n_1, n_2) \in \mathbb{Z}^2_M \tag{III.409}$$

which is fulfilled in case of the free scalar field (III.340) due to its symmetry and $\cos(-t_i) = \cos(t_i)$.

We will now investigate numerically whether the fixed point covariance satisfies the criterion for rotational invariance (III.403). As a sufficient example, we consider the afore-mentioned irrational angle θ, such that $\cos(\theta) = 3/5$. Moreover, we will set the IR cut-off to $R = 1$ for simplicity and without loss of generality the number of spatial dimensions to $D = 2$. As the value of the mass p and the parameter k_0 in (III.351) only

appear in the combination $q^2 := (p^2+k_0^2)\epsilon_M^2$, it suffices to fix the latter one to account for both. Here, we choose $q_1^2 := p^2+k_0^2 = 1$.
First, we present the covariance c_M^* itself for $M=40$ in figure III.8 where the point $m=(0,0)$ lies in the centre. Due to the periodic boundaries the values on the corners do agree with each other. One can see that the next neighbour interactions drop rapidly with $m \in \mathbb{Z}_M^2 = \{0,1,...,M-1\}^2$. The same is true for its Fourier transform $\hat{c}_M^*$. Moreover, the covariance at finite resolution is not invariant under arbitrary rotations, but, heuristically, it appears that the asymmetry could be smoothed out with increasing resolution M.

Next, we consider the quality of the approximant to the rotated covariance as M varies. This approximant, $c_{M\theta}^*$, is the Fourier transform of (III.407) and should agree with the unrotated covariance c_M^* up to a mistake $\mathcal{O}(\epsilon_M^5)$, given the fixed point covariance restores rotational invariance in the continuum. As the same must be true for their Fourier transforms, we consider $\hat{c}_{M\theta}^*$ and $\hat{c}_M^*$ on lattices of different size M and study whether their deviation decays appropriately. Both covariances are of order $\mathcal{O}(\epsilon_M^4)$, hence their *relative deviation* should decay with $\mathcal{O}(\epsilon_M)$:

$$\Delta\hat{c}_M^*(l) := \frac{|\hat{c}_M^*(0,l) - \hat{c}_{M\theta}^*(0,l)|}{\hat{c}_M^*(0,l)} \sim \mathcal{O}(\epsilon_M) \tag{III.410}$$

That it decays indeed fast, is shown in figure III.9 for lattices of size $M=10,40,80$ and 160. Although at low resolution the covariance features a high discrepancy with the approximant $\hat{c}_{M\theta}^*$, the relative deviation $\Delta\hat{c}_M^*$ becomes smaller as the resolution of the spatial manifold increases. Only in a neighbourhood of the centre of the grid, i.e. the point around which we rotate, the approximation fails. But, this neighbourhood shrinks linearly with the resolution M. For $M=160$ the computed covariance already features rotational invariance to a high precision.
To study the decay behaviour of $\Delta\hat{c}_M^*(l)$ further, one could now consider the characteristic function χ_B of a region $B \subset [0,1)^2$ and compare, for different resolutions M, the mean $\overline{\Delta\hat{c}_M}[\chi_B]$ of the relative deviation in this region, i.e. the mean of $\Delta\hat{c}_M^*(l)$ over all $l \in \mathbb{Z}_M^2$ such that $\text{supp}(\chi_l) \subset B$. For example, for $l_0 = (0,2) \in \mathbb{Z}_5^2$ let the support of χ_{l_0} be the region of interest, i.e. on resolution $M_0 = 5$ we have $\overline{\Delta\hat{c}_{M_0}}[\chi_{l_0}] = \Delta\hat{c}_5^*(l_0)$. At any other $M \in 5\mathbb{N}$, we consider the refinement in $\mathbb{Z}_M^2$, i.e. the points $\frac{M}{5}l_0 + \delta$ for $\delta \in [0, M/5-1]^2$. We find that the mean

$$\overline{\Delta\hat{c}_M}[\chi_{l_0}] := \frac{1}{(M/5)^2} \sum_{\delta \in [0,M/5-1]^2} \Delta\hat{c}_M^*(\frac{M}{5}l_0 + \delta) \tag{III.411}$$

is decaying with M^{-1}, see figure III.10 for two examples. It confirms that (III.403), i.e. the condition for rotational invariance, is satisfied up to an error of $\epsilon_M = M^{-1}$ to a very high precision for the considered examples and thus indicates that rotational invariance will be recovered in the continuum.

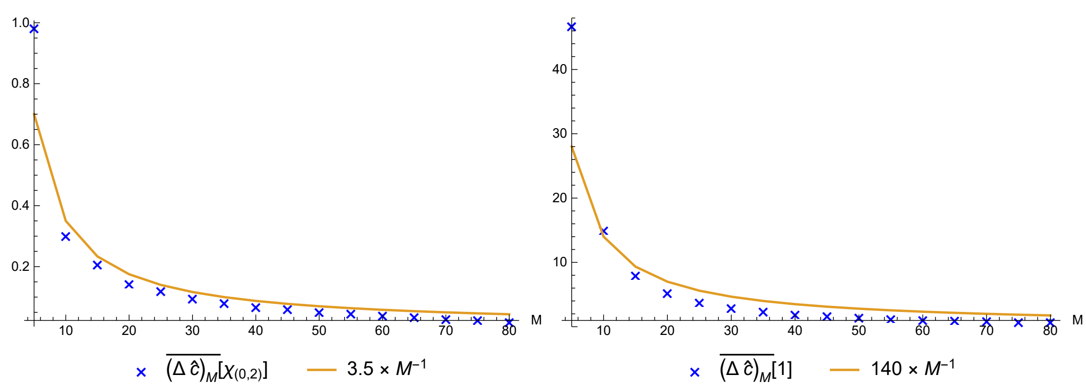

Abbildung III.10: The decay behaviour of the mean $\overline{\Delta\hat{c}_M}[\chi]$ of the relative deviation over a region with characteristic function χ is presented. For two distinct regions, we compute it at different resolutions M. On the left, $\chi_{(0,2)}$ is the characteristic function of this block that can be associated with the point $m_0 = (0,2)$ on resolution $M=5$. The values for $\overline{\Delta\hat{c}_M}[\chi]$ are shown in blue and we approximate the decay behaviour by the function $f(M) = 3.5\ M^{-1}$ (in orange). Similarly, $\chi = 1$ is associated with the whole torus $[0,1)^2$ and is presented on the right. Here, the decay is best approximated by $f(M) = 140 \times M^{-1}$ in orange. These two are arbitrary cases, however we expect the decay to be of this form for each region. This confirms that the decay behaviour is sufficiently fast to account for a rotationally invariant fixed point theory.

Kapitel IV

General Relativity

Some of the best verified theories of modern physics are the two theories of relativity published by Einstein in 1905 and 1916 [15, 16]. Firstly, Special Relativity set the stage by proposing that the speed of light should always be constant in every inertial frame. This presented a radical, yet extremely simple interpretation of the involved formulas other physicists (such as Lorentz) had developed at the end of the 19th century to explain the nature of the universe [226–230].
In consequence, no massive object can be accelerated to the speed of light c. Approaching it, the energy of further acceleration would mostly increase its (relativistic) mass. Hence, only the massless light ray can travel at c, and not even an interaction between particles, like electromagnetism, can exchange information faster. Mathematically, this was achieved by not treating space and time separately - as one was used to - but as a joint object: *spacetime* [231]. By treating time as a new coordinate, special relativity proposes to use the Minkowski metric $\eta_{\mu\nu}$ with diagonal entries $(-c^2, +1, +1, +1)$, which ensures the constant nature of the speed of light. This is known as a metric with Lorentzian signature, a perfect description for a special relativistic world.
The theory of General Relativity (GR) followed when Einstein introduced a possible foundational principle for a theory of gravitation, known as the *equivalence principle*. Einstein stated in 1907 that it assumes *"the complete physical equivalence of a gravitational field and a corresponding acceleration of the reference system"* [232]. A common example is that being at rest in a closed room on the surface of the earth (where we are exposed to a gravitational field) is physically indistinguishable from being inside an accelerated spaceship. Now, since in general accelerated frames the Minkowski metric tensor is transformed into a metric field g, the idea arose that the gravitational field is described by a general Lorentzian metric field g. Of course, gravity must be influenced by and in return influences itself the planets and stars, which are the constituents of the matter in the universe, described by the *energy-momentum tensor* T. This influence is captured in the famous *Einstein field equations*

$$R_{\mu\nu} - \frac{1}{2} R\, g_{\mu\nu} = \kappa\, T_{\mu\nu}, \tag{IV.1}$$

with the constant of proportionality, κ, called the *gravitational coupling constant*. The left-hand side consists of involved functions of the metric g, the object by which we measure distances. "Distance" is a concept that is tightly connected with geometry and thus (IV.1) contains R, the geometric curvature of spacetime. Indeed, these formulas tell us that matter curves spacetime and the gravitational force is nothing more than a purely geometrical object. The mathematical framework needed to deal with geometry will be explained in section *IV.A. Differential Riemannian Geometry*.
To view the consequences of such an identification, let us look at two examples: A light ray is an object of no mass (hence the only object travelling at the maximal velocity c) so it should not be affected by gravitational force as Newton understood it (for him, the gravitational force between two particles was proportional to their mass). Yet, if gravitation in truth changes the curvature of spacetime, it is reasonable to assume that light will follow the curvature and deviate from its original path. This was confirmed by Eddington, who saw during an eclipse that stars near the sun shifted their position to a degree only explicable by the theory of GR [233]. Another example (which we will come back to later in *IV.D. Example: Cosmological Models*) is the Friedmann-Lemaître-Robertson-Walker (FLRW) model for our universe [20–32]. These special solutions of (IV.1) allow for various possibilities of the shape of the universe. For example, it could be looking like the three-dimensional pendant to the surface of a sphere. A sphere, as an object with positive curvature, is drastically different from an infinitely spread plane. E.g., launching a rocket which travels always in the same direction would allow the rocket to return automatically back to the point it started from only in the first case.
Having ascertained that geometry describes how the gravitational effects in our universe look like, we will start

to investigate the Einstein field equations further. An important property of them is that their physical effects are independent of the coordinates. This is a rather intuitive property: imagine two people looking at the same experiment under different angles. Although what they individually see differs, the physical observations they describe will be the same. Since GR is a theory defined on a spacetime, we point out that this works also for the time axis: if everything stays the same and we consider the same observer, it doesn't matter whether we measure an observable, i.e. conduct an experiment, with respect to clocks running at different speeds. Switching between two frames of observation is commonly referred to as a change of coordinate systems or a *diffeomorphism*. Hence, GR turns out to be *diffeomorphism invariant*.

However, the formulation of GR also comes with a drawback. Namely, it could allow for solutions featuring *closed causal curves*, i.e. time-travel possibilities. We want to avoid those possibilities and ask for situations where we have a well posed initial value formulation. This means that the spacetime is predictable knowing the initial data of the metric on a spacelike hypersurface σ. Then, one can show that our whole spacetime looks like $\sigma \times \mathbb{R}$ where the real line takes the role of label for the spatial hypersurfaces [40, 234, 235]. Hence, we might call it coordinate time in the following.

This assumption - a physically sensible one - allows us to rewrite (IV.1) in its initial value formulation. This will be done in section *IV.B Hamiltonian Formulation of General Relativity*, where we will derive the corresponding Hamiltonian theory [56], i.e. we will find a function $H(t)$ with which we can compute how all observables evolve in the coordinate time t. In other words, this function is a Hamiltonian generating translation in time. However, we had established that GR is invariant under diffeomorphisms, hence especially under time translations. But then the generator should vanish. Hence, if we are discussing a solution for GR, it must necessarily be true that $H(t) = 0$ for all t. And indeed, we will see that the Hamiltonian is constrained to vanish. This is a rather unsatisfactory realisation often called *the problem of time*. A vanishing Hamiltonian should imply that there is no time evolution of physical observables and everything will remain "frozen", which is in drastic contrast with our everyday observations.

To resolve this seemingly contradicting result, we must look at the detailed structure of the Hamiltonian, which has two constituents

$$H(t) \;=\int_{\sigma(t)} d^3x \;(\; H_{\text{geometry}}(x,t) + H_{\text{matter}}(x,t)\;) \;=\; 0, \tag{IV.2}$$

where the first term evolves only the gravity part, which we remember to be just geometrical effects, and the second contains the interaction of gravity with the matter of our universe. As such, it derives from the right-hand side of the equation (IV.1). Assume for simplicity that we would have a universe where the only matter appearing is some simple clock. Whenever the clock ticks the matter Hamiltonian changes and, since the whole of (IV.2) must be zero, consequently the geometry *must* change. So, we see that time evolution happens if we can relate it to a certain clock measuring it. This so-called *relational formalism* faithfully describes how we experience time in reality: we cannot grasp time itself, but we can observe how far the pointer of a clock has moved during a measurement. We should not give too much weight to the coordinate time t, but rather we should label evolution by some value of a suitable *clock matter field*, which we will call ϕ.

A question, giving rise to a lot of debate, is what exactly the Hamiltonian for the clock field should look like. Many proposals exist, which can be applied in various applications. We will present here one, which is very often used in the context of isotropic spacetimes: In principle, everything can work as a clock and thus the galaxies, thinly spread in the universe, with all the star formations happening inside them make perfect candidates. However, they are far too complicated to be used for actual computations by which we would like to describe the evolution of our universe. So, one must find a simplification that is feasible and yet possesses the key features of a "galaxy clock". For example, studying the sky our observable universe looks extremely *isotropic*, i.e. it is symmetric in the sense that in every direction we see approximately the same density of galaxies. This is also visible in the famous *cosmic microwave background*, which is isotropic to roughly one part in 100.000 [20, 21]. We conclude that we occupy no exceptional point in space, a concept which has become known as the *cosmological principle*. Hence, the whole universe should look isotropic everywhere and thus also our clock field should obey this symmetry. When studying isotropic spacetimes we will hence, among the many approximations which have proven themselves useful, restrict our attention to a homogeneously spread, free massive scalar field, which in the literature is also called *Klein-Gordon field* and which we have already encountered in the previous chapters. Using it as a clock field we compute an explicit example for our universe at large scales in *IV.D. Example: Cosmological Models*.

This clock field has proven useful for many cosmological applications, for example a generalisation thereof is one of the standard techniques to describe inflation [236]. A remarkable property of this scalar field clock for the case of an isotropic universe is that, with each passing instance of the coordinate time t, the value of the clock ϕ will strictly increase, which is indeed a useful property for a clock. However, it also means when looking at (IV.2) that with a changing matter field the geometry part must change as well, hence excluding a stable, static universe, which is isotropic. This is in agreement with today's observations of the galaxies drifting apart. As the universe expands, this implies in consequence that at some point in the far past there must have been a moment where the universe was infinitesimal small. All matter was condensed in a single point with infinite energy density, the famous *Big Bang singularity*!

A singularity, like this one, is an indication that the theory left its domain of validity. In particular, we would expect that the epoch where the scale factor of the universe was very small is in truth dominated by quantum effects. Hence, to resolve the singularity we will discuss a possible candidate for a theory of quantum gravity in the last chapter of this thesis, *V. Loop Quantum Gravity*. For the approach discussed there, it is necessary to express GR in new variables which will be introduced in *IV.C.1. Ashtekar-Barbero Variables*. Instead of using the metric g itself, Ashtekar built two functions containing it, $(A^I_a,\ E^b_J)$. These are covector and vector fields on σ, indexed by $I, J = 1, ...3$, which form a *canonical pair* [53–55], i.e. their Poisson bracket is proportional to a Dirac δ distribution:

$$\{\ A^I_a(x)\ ,\ E^b_J(y)\ \} = \frac{\kappa\beta}{2}\delta^I_J\delta^b_a\delta^{(3)}(x,y). \tag{IV.3}$$

The constant $\beta \neq 0$ can be any non-vanishing complex number, labelling a whole family of possible choices. Indeed, under certain constraints (i.e. vanishing of a specific function $G_J(A^I_a, E^J_b) = 0$ called *Gauss constraint*) this formulation becomes equivalent to GR. Moreover, the Ashtekar-Barbero variables have the form of a *gauge theory*, i.e. we can now use the whole mathematical toolbox known from other gauge theories like, e.g. electromagnetism and quantum chromodynamics. As mentioned, we will see the advantage of this especially in the last chapter of this thesis, where we will aim at a possible definition of a theory of *Quantum Gravity*. Thanks to the formulation of Ashtekar, this ambitious program can be carried out in exact analogy to the experimentally verified quantum gauge field theories.

IV.A Differential Riemannian Geometry

In this chapter we collect the basic notions from differential geometry. Textbooks covering further details are for example [237, 238].

IV.A.1 Manifolds and Tensors

Definition IV.A.1 (Manifolds, hypersurfaces)**.** *An m-dimensional C^k manifold $\mathcal{M}$ is a topological space, i.e. a set of points, with a collection of open subsets $(U_I)_{I\in\mathcal{I}}$ (with arbitrary index set $\mathcal{I}$) such that*

1. *$\mathcal{M} = \cup_{I\in\mathcal{I}} U_I$, i.e. the subsets form an open cover of $\mathcal{M}$.*
2. *There exists a homeomorphism $x_I : U_I \to x_I(U_I) \subset \mathbb{R}^m$ called* chart.
3. *For all $I, J \in \mathcal{I}$ with $U_I \cap U_J \neq 0$, the map $x_{I\to J} := x_J \circ x_I^{-1} : x_I(U_I \cap U_J) \to x_J(U_I \cap U_J)$ is a C^k map between open subsets, i.e. $x_{I\to J}$ is k-times continuously differentiable.*

A subset $\sigma \subset \mathcal{M}$ of an m-dimensional manifold $\mathcal{M}$ is called a hypersurface *if*

1. *σ is equipped with the induced (subspace) topology of $\mathcal{M}$, i.e. its open sets are given by $V_I := \sigma \cap U_I$ where $U_I \subset \mathcal{M}$ are open.*
2. *The dimension of σ is $\dim\sigma = m - 1$ and for $x'_I := x_I\ |_{V_I}$ the map $x'_{I\to J} := x'_J \circ {x'_I}^{-1}$ is C^k.*
3. *There exists an* embedding *map $\psi : \sigma \to \mathcal{M}$ such that $\psi(V_I)$ is open $\forall V_I$ and $\sigma \to \psi(\sigma)$ is an injection, i.e. not self-intersecting.*

In the following we consider functions $f : \mathcal{M} \to \mathbb{C}$ which are smooth, i.e. $f \in C^\infty$, iff $f \circ x_I^{-1}$ is smooth on $x_I(U_I) \subset \mathbb{R}^m$.

Definition IV.A.2 (Vector fields, one-forms)**.** *A smooth* vector field *v on $\mathcal{M}$ is a linear map*

$$\begin{aligned} v : C^\infty(\mathcal{M}) &\to C^\infty(\mathcal{M}) \\ f &\mapsto v[f], \end{aligned} \tag{IV.4}$$

such that $v[fg] = v[f]g + fv[g]$ and annihilates constants.
The space of all smooth vector fields shall be denoted by $T^1(\mathcal{M})$, on which we define the linear maps

$\omega : T^1(\mathcal{M}) \to C^\infty(\mathcal{M})$, which are called one-forms*. Calling $T_1(\mathcal{M})$ the space of all one-forms we define the* exterior derivative *d as the map*

$$\begin{aligned} d : C^\infty &\to T_1(\mathcal{M}) \\ f &\mapsto df \;\; \text{s.t. } df[v] := v[f] \end{aligned} \tag{IV.5}$$

for all $v \in T^1(\mathcal{M})$.

In any chart (U, x) we can consider at each p the components $x^\nu := x(p)^\nu \in \mathbb{R}^m$ and the special vector fields ∂_μ defined by the condition

$$(\partial_\mu x^\nu)(p) = \delta^\nu_\mu. \tag{IV.6}$$

Indeed the ∂_μ form a basis of $T^1(\mathcal{M})$ as for all v one can express $v(p) = v^\mu(x)\partial_\mu$, which is independent of the chart in use. Similar we find a basis for $T_1(\mathcal{M})$ as dx^ν so that

$$(dx^\nu(\partial_\mu))(p) = \delta^\nu_\mu. \tag{IV.7}$$

In particular we find for all $f \in C^\infty(\mathcal{M})$

$$df = (\partial_\mu f) dx^\mu \tag{IV.8}$$

Definition IV.A.3 (Diffeomorphisms)**.** *Let $(U_I, x_I)_{I\in\mathcal{I}}$ be the charts of an m-dimensional manifold $\mathcal{M}$. A map $\varphi : \mathcal{M} \to \mathcal{M}$ is called C^∞ iff for each $I, J \in \mathcal{I}$ the map $x_I \circ \varphi \circ x_J^{-1}$ is well defined and also C^∞. If φ is C^∞ and has an inverse which is also C^∞ we call it a* diffeomorphism*. The diffeomorphisms of a manifold $\mathcal{M}$ form a group which is denoted by* Diff$(\mathcal{M})$*.*

Definition IV.A.4 (Tensor fields, n-forms)**.** *An (a, b)-*tensor field *$t : T_1(\mathcal{M})...T_1(\mathcal{M})\times T^1(\mathcal{M})...T^1(\mathcal{M}) \to C^\infty(\mathcal{M})$ is a functional, linear in each entry, which writes explicitly*

$$t(p) = t^{\mu_1\cdots\mu_a}_{\nu_1\ldots\nu_b}(p)\;(\partial_{\mu_1} \otimes ... \otimes \partial_{\mu_a} \otimes dx^{\nu_1} \otimes ... \otimes dx^{\nu_b})(p) \tag{IV.9}$$

where $t^{\mu_1\cdots\mu_a}_{\nu_1\ldots\nu_b} \in \mathbb{R}$ and transforms under a change of coordinate systems x_I, x_J according to

$$(t_I)^{\mu_1\cdots\mu_a}_{\nu_1\ldots\nu_b}(x_I(p)) = (\varphi^*_{I\to J} t_J)^{\mu_1\cdots\mu_a}_{\nu_1\ldots\nu_b}(x_I(p)) := (t_J)^{\mu'_1\cdots\mu'_a}_{\nu'_1\ldots\nu'_b}(x_J(p)) \left(\prod_{k=1}^{a} \frac{\partial x_I^{\mu_k}(p)}{\partial x_J^{\mu'_k}(p)}\right) \left(\prod_{l=1}^{b} \frac{\partial x_J^{\nu'_l}(p)}{\partial x_I^{\nu_l}(p)}\right), \tag{IV.10}$$

where $\varphi^*_{I\to J}$ is called the pull-back *of a diffeomorphism*[1] *between both charts, such that $x_J = \varphi_{I\to J} \circ x_I$. The space of all tensor fields of type (a, b) is denoted as $T^a_b(\mathcal{M})$.*
The special case of $\omega \in T^0_n(\mathcal{M})$ is called an n-form *iff its component functions $\omega_{\nu_1\ldots\nu_n}$ are totally skew. On their space, $\Omega_n(\mathcal{M})$, we define the* exterior product *by*

$$\begin{aligned} \wedge : \Omega_{k_1}(\mathcal{M}) \times \Omega_{k_2}(\mathcal{M}) &\to \Omega_n(\mathcal{M}) \\ \omega_1 \times \omega_2 &\mapsto (\omega_1 \wedge \omega_2) \end{aligned} \tag{IV.11}$$

such that

$$(\omega_1 \wedge \omega_2)(v_1...v_n) := \frac{1}{k_1!k_2!} \sum_{\pi\in S_n} sgn(\pi)\omega_1(v_{\pi(1)}...v_{\pi(k_1)})\omega_2(v_{\pi(k_1+1)}...v_{\pi(n)}) \tag{IV.12}$$

with $n = k_1 + k_2$ and $\pi \in S_n$ is a permutation. The exterior derivative *$d : \Omega_n(\mathcal{M}) \to \Omega_{n+1}(\mathcal{M})$ is given by*

$$d\omega(v_0, ...v_n) = \sum_{k=0}^{n} (-1)^k v_k[\omega(v_0, ..., \not{v}_k, ..., v_n)] + \sum_{k\le l=0}^{n} (-1)^{k+l}\omega([v_k, v_l], v_0...\not{v}_k, ..., \not{v}_l, ..., v_n), \tag{IV.13}$$

where $[v, w][f] := v[w[f]] - w[v[f]]$.

The definition of d is in agreement with (IV.5) and implies moreover $d(\omega_1 \wedge \omega_2) = d\omega_1 \wedge \omega_2 + (-1)^{k_1}\omega_1 \wedge d\omega_2$ for $\omega_i \in \Omega_i(\mathcal{M})$, $d\omega_m = 0$ if $m = \dim \mathcal{M}$ and $d^2 = 0$.
In the following, if a tensor field $t \in T^a_b(\mathcal{M})$ is defined globally we will employ the abstract index notation $t^{\mu_1\cdots\mu_a}_{\nu_1\ldots\nu_b}$ and drop the index I of the locally defined component functions.

[1] In physics jargon this is called a *passive* diffeomorphism, i.e. a map between some of the various coordinate systems. Later on, the phrase *diffeomorphism invariance* of e.g. an action will mean that such smooth changes of coordinates do not affect the value of the action functional.

IV.A.2 Metric and Spacetime

Definition IV.A.5 (Metric)**.** *A* metric tensor field $g \in T_2^0(\mathcal{M})$ *is a symmetric, non-degenerate tensor field*[2]. *As* n*, the number of negative eigenvalues is independent of any chosen basis we call the metric of* Lorentzian signature *if* $n = 1$ *and of* Euclidian signature *if* $n = 0$*. We call the pair* $(\mathcal{M}, g)$ *a* spacetime*.*

As g is non-degenerate there exists its inverse g^{-1} whose components will be simply denoted $g^{\mu\nu}$. Hence $g^{\nu\mu} g_{\mu\rho} = \delta^\nu_\rho$. For a vector v^μ we will adopt the notation $v_\mu := g_{\mu\nu} v^\nu$ for its dual, and similar for tensor fields.

Definition IV.A.6 (Covariant Differential)**.** *A map* $\nabla' : T_b^a(\mathcal{M}) \to T_{b+1}^a(\mathcal{M})$, $t^{\mu_1 \dots \mu_a}_{\nu_1 \dots \nu_b} \mapsto \nabla'_{\nu_{b+1}} t^{\mu_1 \dots \mu_a}_{\nu_1 \dots \nu_b}$ *is called* affine connection *or* covariant differential *if it obeys the following properties:*

1. *Linearity: for all* $t_1, t_2 \in T(\mathcal{M})$ *and* $z_1, z_2 \in \mathbb{C}$*:*
$$\nabla'(z_1 t_1 + z_2 t_2) = z_1 \nabla' t_1 + z_2 \nabla' t_2. \tag{IV.14}$$
2. *Leibniz rule: for all* $t_1, t_2 \in T(\mathcal{M})$*:*
$$\nabla' \left(t_1 \otimes t_2\right) = (\nabla t_1) \otimes t_2 + t_1 \otimes (\nabla t_2). \tag{IV.15}$$
3. *Commutativity with contraction: for all* $t \in T(\mathcal{M})$*:*
$$\nabla'(t[..,\omega,..,v,..]) = (\nabla' t)[..,\omega,..,v,..] + ... + t[..,\nabla'\omega,..,v,..] + ... + t[..,\omega,..,\nabla' v,..] + ... \tag{IV.16}$$
4. *Consistency with the notion of tangent vectors as directional derivatives on scalar fields: for all* $f \in C^\infty$ *and* $v \in T^1(\mathcal{M})$*:*
$$v[f] = v^\mu \nabla'_\mu f\ . \tag{IV.17}$$
5. *Torsion free*[3]*: for all* $f \in C^\infty$*:*
$$\nabla'_\mu \nabla'_\nu f = \nabla'_\nu \nabla'_\mu f\ . \tag{IV.18}$$

The existence of such covariant derivatives is found by considering $(\nabla^0 t)^{\mu_1 \cdots \mu_a}_{\nu_{b+1} \nu_1 \dots \nu_b} := \partial t^{\mu_1 \cdots \mu_a}_{\nu_1 \dots \nu_b} / \partial x^{\nu_{b+1}}$, which obeys all five criteria. However, uniqueness of these operators is in general not given. We will define the components of ∇' acting on a vector field ∂_μ as

$$\Gamma^\rho_{\mu\nu} \partial_\rho := \nabla'_\mu \partial_\nu\ . \tag{IV.19}$$

It follows then from $\nabla'(\delta_\mu[x^\nu]) = \nabla'(dx^\nu(\partial_\mu)) = 0$ that $\nabla'_\mu dx^\nu = -\Gamma^\nu_{\mu\rho} dx^\rho$ and combined with (IV.17) we can write the explicit components of (IV.16) as

$$\nabla'_\mu t^{\mu_1 \dots \mu_a}_{\nu_1 \dots \nu_b} := \partial_\mu [t^{\mu_1 \dots \mu_a}_{\nu_1 \dots \nu_b}] + \sum_{k=1}^{a} \Gamma^{\mu_k}_{\mu\rho} t^{\mu_1 \dots \not{\mu}_k \rho \dots \mu_a}_{\nu_1 \dots \nu_b} - \sum_{l=1}^{b} \Gamma^{\rho}_{\mu\nu_l} t^{\mu_1 \dots \mu_a}_{\nu_1 \dots \not{\nu}_l \rho \dots \nu_b} \tag{IV.20}$$

Definition IV.A.7 (Curves, tangential vectors)**.** *A smooth* curve *in* $\mathcal{M}$ *is a* C^∞ *map* $c : [a,b] \subset \mathbb{R} \to \mathcal{M}$, $s \mapsto c(s)$*. For each* c *one may define the* tangential vector field $v_{c(s)}$ *along* c *as*

$$v_{c(s)}[\ .\ ] := \left(\frac{dx^\mu_I(s')}{ds'}\right)_{s'=s} \partial_\mu(\ .\ )\ |_{x_I(c(s))} \tag{IV.21}$$

Given $p := c(0)$ we would call c the integral curve of v through p. Conversely, given a vector field v and a point p there exists a unique integral curve c^v_p of v through p and we assign to it a one-parameter group of diffeomorphisms

$$\varphi^v_s(p) := c^v_p(s)\ . \tag{IV.22}$$

[2] In physics jargon one uses sometimes the notation $ds^2 = g = g_{\mu\nu} dx^\nu \otimes dx^\nu$ when expressing the metric in a basis and calls ds^2 the *line element*.

[3] This condition is sometimes dropped. However, when talking about GR, it can be used to ensure that one can assign for a given metric g a unique (torsion-free) connection ∇, which is compatible with respect to g, i.e. $\nabla g = 0$ (see theorem IV.A.1).

Definition IV.A.8 (Lie derivative)**.** *Given a smooth vector field v, we define the* Lie derivative *of a tensor $t \in T^a_b(\mathcal{M})$ to be*

$$(\mathcal{L}_v t)(p) := \left(\frac{d}{ds}\right)_{s=0} ((\varphi^v_s)^* t)(p) \; . \tag{IV.23}$$

A tensor field t is said to be invariant under a diffeomorphism φ iff $\varphi^* t = t$ and symmetric under the flow of v iff $\mathcal{L}_v t = 0$.

Since $\mathcal{L}_v$ is linear in v we consider for the moment the coordinate system x_I in which $v^a = \partial/\partial x^1_I$, in which (IV.23) explicitly reads

$$(\mathcal{L}_v t)^{\mu_1\dots\mu_a}_{\nu_1\dots\nu_b} = \frac{\partial}{\partial x^1_I} t^{\mu_1\dots\mu_a}_{\nu_1\dots\nu_b} \; . \tag{IV.24}$$

Thus, for a vector field w it follows:

$$\mathcal{L}_v w^\mu = \frac{\partial}{\partial x^1_I} w^\mu = v^\nu \partial_\nu w^\mu - w^\nu \partial_\nu v^\mu = [v,w]^\mu \tag{IV.25}$$

which is independent of the choice x_I. And consequently also $\mathcal{L}_v f = v[f]$ for $f \in C^\infty$, which implies for a one-form ω via Leibniz rule

$$w^\mu \mathcal{L}_v \omega_\mu = \mathcal{L}_v(\omega_\mu w^\mu) - \omega_\mu [v,w]^\mu = v[\omega_\mu w^\mu] - \omega_\mu v^\nu \nabla'_v w^\mu + \omega_\mu w^\nu \nabla'_\nu v^\mu = w^\mu(v^\nu \nabla'_\nu \omega_\mu + \omega_\nu \nabla'_\mu v^\nu) \tag{IV.26}$$

which has to be true for all w and hence uniquely determines $\mathcal{L}_v \omega$. Continuing in this manner inductively we find:

Corollary IV.A.1. *Let $t \in T^a_b(\mathcal{M})$ and $v \in T^1(\mathcal{M})$ then for* any *covariant differential ∇' it holds:*

$$\mathcal{L}_v t^{\mu_1\dots\mu_a}_{\nu_1\dots\nu_b} = v^\mu \nabla'_\mu t^{\mu_1\dots\mu_a}_{\nu_1\dots\nu_b} - \sum_{k=1}^{a} t^{\mu_1\dots\not{\mu}_k\mu\dots\mu_a}_{\nu_1\dots\nu_b} \nabla'_\mu v^{\mu_k} + \sum_{l=1}^{b} t^{\mu_1\dots\mu_a}_{\nu_1\dots\not{\nu}_l\mu\nu_b} \nabla'_{\nu_k} v^\mu \tag{IV.27}$$

Given a covariant derivative the notion of parallel transport of a tensor t along a curve with tangent v is

$$v^\mu \nabla'_\mu t^{\mu_1\dots\mu_a}_{\nu_1,\dots,\nu_b} = 0 \; . \tag{IV.28}$$

Concretely, for a vector $w^\mu(p)$ this means $v^\mu \partial_\mu w^\nu + v^\mu \Gamma^\nu_{\mu\rho} w^\rho = 0$, which is an ordinary differential equation. Hence, given $w^\mu(p = c(0))$ this defines for all parameters s of the curve uniquely $w^\mu(c(s))$, the parallel transported vectors[4].

Theorem IV.A.1 (Levi-Civita Connection)**.** *Given a spacetime $(\mathcal{M}, g)$ there exists a unique (torsion-free) metric-compatible covariant derivative ∇, i.e. $\nabla g = 0$. We call it the* Levi-Civita connection *and its components the* Christoffel symbols*, which are given by*

$$\Gamma^\rho_{\mu\nu} = \frac{1}{2} g^{\rho\sigma}(\partial_\mu g_{\nu\sigma} + \partial_\nu g_{\mu\sigma} - \partial_\sigma g_{\mu\nu}) \tag{IV.29}$$

Proof. First we use the torsion-freeness on $\nabla'_\mu \nabla'_\nu f = \partial_\mu \partial_\nu f - \Gamma^\rho_{\mu\nu} \nabla'_\rho f$ to get

$$2\Gamma^\rho_{[\mu\nu]} \nabla'_\rho f = [\partial_\mu, \partial_\nu] f =: c^\rho_{\mu\nu} \partial_\rho f = c^\rho_{\mu\nu} \nabla'_\rho f \tag{IV.30}$$

displaying the symmetry property $\Gamma^\rho_{\mu\nu} = \Gamma^\rho_{\nu\mu}$ for a coordinate system. Requiring $\nabla g = 0$ implies by (IV.20)

$$0 = \nabla_\rho g_{\mu\nu} = \partial_\rho g_{\mu\nu} - \Gamma^\sigma_{\rho\mu} g_{\sigma\nu} - \Gamma^\sigma_{\rho\nu} g_{\mu\sigma} \tag{IV.31}$$

$$\Leftrightarrow \Gamma_{\nu\rho\mu} + \Gamma_{\mu\rho\nu} = \partial_\rho g_{\mu\nu} \tag{IV.32}$$

We switch in (IV.32) the indices $\rho \leftrightarrow \mu$ and add it to itself and subtract moreover a cyclic permutation of the indices of (IV.32), too. Using (IV.30) with $\Gamma^\rho_{\mu\nu} = \Gamma^\rho_{(\mu\nu)} + \Gamma^\rho_{[\mu\nu]}$

$$2\Gamma_{\rho\mu\nu} = \partial_\mu g_{\nu\rho} + \partial_\nu g_{\mu\rho} - \partial_\rho g_{\mu\nu} - c_{\rho\mu\nu} + c_{\nu\mu\rho} + c_{\mu\rho\nu} \tag{IV.33}$$

Dividing by two and multiplying with the inverse metric gives (IV.29), if we are in a coordinate system (where $c^\rho_{\mu\nu} = 0$ for all μ, ν, ρ). □

[4]Sometimes, one wants that the scalar product of two vectors at a given point, i.e. $g_{\mu\nu} w^\mu \tilde{w}^\nu$, does not change if parallelly transported along a curve with tangent field v. Thus $w^\mu, \tilde{w}^\nu$ are separately transported via (IV.28) and we require

$$v^\rho \nabla'_\rho (g_{\mu\nu} w^\mu \tilde{w}^\nu) = 0$$

After applying the Leibniz rule, one sees that is this true for any curve if only if $\nabla'_\rho g_{\mu\nu} = 0$. This motivates to consider the following Levi-Civita connection.

IV.A.3 Riemann Curvature

Definition IV.A.9 (Riemann curvature, Ricci scalar)**.** *Given a spacetime* $(\mathcal{M}, g)$ *and its metric-compatible Levi-Civita connection* ∇ *the* Riemann curvature tensor *in* $T^1_3(\mathcal{M})$ *is defined by its components*

$$R^{\sigma}_{\ \mu\nu\rho} = -2\partial_{[\mu}\Gamma^{\sigma}_{\nu]\rho} + 2\Gamma^{\lambda}_{\rho[\mu}\Gamma^{\sigma}_{\nu]\lambda} \, . \tag{IV.34}$$

The following contractions are called the Ricci tensor *and* Ricci scalar *respectively*

$$R_{\mu\rho} = R^{\sigma}_{\ \mu\sigma\rho}, \qquad\qquad R = g^{\mu\rho}R_{\mu\rho} \, . \tag{IV.35}$$

The action of the Riemann curvature tensor on one-forms ω can be written more compactly as

$$\begin{aligned}2\nabla_{[\mu}\nabla_{\nu]}\omega_\rho = 2\nabla_{[\mu}(\partial_{\nu]}\omega_\rho - \Gamma^{\sigma}_{\nu]\rho}\omega_\sigma) = -2\Gamma^{\sigma}_{\rho[\mu}\partial_{\nu]}\omega_\sigma - 2\partial_\mu(\Gamma^{\sigma}_{\nu]\rho}\omega_\sigma) + 2\Gamma^{\lambda}_{\rho[\mu}\Gamma^{\sigma}_{\nu]\lambda}\omega_\sigma = \\ = (-2\partial_{[\mu}\Gamma^{\sigma}_{\nu]\rho} + 2\Gamma^{\lambda}_{\rho[\mu}\Gamma^{\sigma}_{\nu]\lambda})\omega_\sigma = R^{\sigma}_{\ \mu\nu\rho}\omega_\sigma \, ,\end{aligned} \tag{IV.36}$$

where we have used several times the beforehand established symmetry property $\Gamma^{\rho}_{[\mu\nu]} = 0$. Thus for any vectorfield v follows by the Leibniz property

$$0 = 2\nabla_{[\mu}\nabla_{\nu]}(\omega_\rho v^\rho) = 2\omega_\rho\nabla_{[\mu}\nabla_{\nu]}v^\rho + 2v^\rho\nabla_{[\mu}\nabla_{\nu]}\omega_\rho = \omega_\rho(2\nabla_{[\mu}\nabla_{\nu]}v^\rho + v^\rho R^{\sigma}_{\ \mu\nu\rho}) \tag{IV.37}$$

which gives the general action of $R^{\sigma}_{\ \mu\nu\rho}$ on vector fields and, by using metric compatibility of ∇, this yields finally the following symmetry property:

$$0 = \nabla_{[\mu}\nabla_{\nu]}g_{\rho\sigma}v^\rho\tilde{v}^\sigma = v^\rho\tilde{v}^\sigma\nabla_{[\mu}\nabla_{\nu]}g_{\rho\sigma} - g_{\rho\sigma}v^\rho R^{\sigma}_{\ \mu\nu\lambda}\tilde{v}^\lambda - g_{\rho\sigma}\tilde{v}^\sigma R^{\rho}_{\ \mu\nu\lambda}v^\lambda = v^\rho\tilde{v}^\lambda(g_{\rho\sigma}R^{\sigma}_{\ \mu\nu\lambda} + g_{\sigma\lambda}R^{\sigma}_{\ \mu\nu\rho}) \, . \tag{IV.38}$$

Moreover, we can relate $R^{\sigma}_{\ \mu\nu\rho}$ with the parallel transport along curves. Consider two commuting vector fields k^1, k^2, i.e. tangents of some coordinate system x^1_S, x^2_S, and the integral curves $c^{k^1}_p, c^{k^2}_p, c^{k^1}_{c^{k^2}(\Delta x^2)}, c^{k^2}_{c^{k^1}(\Delta x^1)}$ with $\Delta x^1, \Delta x^2 \in \mathbb{R}$. Hence e.g. along $c^{k_1}_p$ we find $x^2_S = 0$. For all one-forms ω we transport the vector $v^\nu(p)$ along the loop formed by those curves. The displacement along the first segment is to first order in Δx^1:

$$\begin{aligned}v^\mu\omega_\mu(\Delta x^1, 0) - v^a\omega(0,0) \approx \Delta x^1_S(\frac{\partial}{\partial x^1_S}v^a\omega_a)(\Delta x^1/2_S, 0) = \Delta x^1_S((k^1)^\mu\nabla_\mu v^\mu\omega_\nu)(\Delta x^1_S/2, 0) = \\ = \Delta x^1_S(v^\nu(k^1)^\mu\nabla_\mu\omega_\nu)(\Delta x^1_S/2, 0) \, ,\end{aligned} \tag{IV.39}$$

where we used in the last step the fact that we are parallel transporting v, (IV.28). Similarly, one finds that to first order in Δx^2_S

$$\begin{aligned}(v^\nu(k^1)^\mu\nabla_\mu\omega_\nu)(\Delta x^1_S/2, \Delta x^2_S) = \\ = v^\nu(k^1)^\mu\nabla_\mu\omega_\nu(\Delta x^1_S/2, 0) + \Delta x^2_S((k^2)^\mu\nabla_\mu v^\nu(k^2)^{\mu'}\nabla_{\mu'}\omega_\nu)(\Delta x^1_S/2, \Delta x^2_S/2)\end{aligned} \tag{IV.40}$$

Now, the k^1, k^2 were chosen such that they commute with each other. It follows that δv^a, the displacement of the vector v^a after going along the whole loop, reads:

$$\delta(v^a\omega_a) = \Delta x^1_S\Delta x^2_S v^\nu(k^1)^\mu(k^2)^{\mu'}\nabla_{[\mu}\nabla_{\mu']}\omega_\nu \tag{IV.41}$$

which has to be true for all ω and thus displays a connection between the displacement of δv^a and $R^{\sigma}_{\ \mu\nu\rho}$. Hence vanishing of the Riemann curvature is the condition for parallel transport of vectors along a curve to be trivial[5]. If that is the case, we say that the connection ∇ is flat.

IV.B Hamiltonian Formulation of General Relativity

We now turn to vacuum[6] GR, which we will define on some orientable, globally-hyperbolic[7] 4-dimensional manifold $\mathcal{M} \cong \mathbb{R} \times \sigma$ with $\partial\mathcal{M} = \emptyset$ and whose degrees of freedom are given by the components of the metric tensor field and whose action is the *Einstein-Hilbert action* [16, 239].

[5] Equivalently the (later-introduced) holonomy (IV.152) of the curve is trivial

[6] If one would add a matter Lagrangian $\mathcal{L}_M$ to the Einstein-Hilbert action, one obtains on the right hand side of (IV.43) the corresponding energy density tensor $8\pi G T_{\mu\nu}/c^4$.

[7] This means there exists a Cauchy surface σ, i.e. a hypersurface such that g_ν is completely determined by the initial conditions on σ. By Gerochs splitting theorem follows automatically that $\mathcal{M} \cong \mathbb{R} \times \sigma$, i.e. we have not neglected anything with this assumption [40, 234, 235].

IV.B.1 Einstein-Hilbert action

Theorem IV.B.1 (Einstein-Hilbert action, Einstein field equation)**.** *The field theory of the metric tensor described by the* Einstein-Hilbert-action

$$S_{EH} = \frac{1}{\kappa} \int_{\mathcal{M}} d^4x \; R \; \sqrt{-\det(g_{\mu\nu})} \tag{IV.42}$$

where $\kappa = 16\pi G c^{-4}$ is the gravitational coupling constant, can be cast into the following set of differential equations, called Einstein field equations

$$R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} = 0 \tag{IV.43}$$

Proof. We start by calculating the variation of the Lagrangian ($g := \det(g_{\mu\nu})$):

$$\delta(R\sqrt{g}) = \sqrt{-g} g^{\mu\nu} (\delta R_{\mu\nu}) + \sqrt{-g} R_{\mu\nu} \delta g^{\mu\nu} + R \delta \sqrt{-g} \tag{IV.44}$$

As one can show, by expressing the determinant as contractions with the Levi-Civita symbol, it holds $\delta g = g g^{\mu\nu} \delta g_{\mu\nu}$ and thus

$$\delta\sqrt{-g} = \frac{i}{2\sqrt{g}} \delta g = \frac{1}{2} \sqrt{-g} (g^{\mu\nu} \delta g_{\mu\nu}) = -\frac{1}{2} \sqrt{-g} (g_{\mu\nu} \delta g^{\mu\nu}) \tag{IV.45}$$

Since $\delta\Gamma^\rho_{\mu\nu}$ is the difference of two connections it is a tensor. Hence, one can compute

$$\nabla_\mu (\delta\Gamma^\rho_{\nu\sigma}) = \partial_\mu \Gamma^\rho_{\nu\sigma} + \Gamma^\rho_{\mu\lambda} \delta\Gamma^\lambda_{\nu\sigma} - \Gamma^\lambda_{\mu(\nu} \delta\Gamma^\rho_{\sigma)\lambda} \tag{IV.46}$$

and it follows

$$\nabla_\mu (\delta\Gamma^\rho_{\nu\sigma} - \nabla_\nu (\delta\Gamma^\rho_{\mu\sigma}) = 2\delta(\partial_{[\mu} \Gamma^\rho_{\nu]\sigma} + \Gamma^\rho_{\lambda[\mu} \delta\Gamma^\lambda_{\nu]\sigma} - \Gamma^\lambda_{\sigma[\mu} \delta\Gamma^\rho_{\nu]\lambda}) = \delta R^\rho_{\sigma\mu\nu} \tag{IV.47}$$

Moreover, we can replace the density one vector field divergence ∇_μ with ∂_μ and get

$$\sqrt{-g} g^{\mu\nu} \delta R^\rho_{\mu\rho\nu} = \sqrt{-g} \nabla_\rho (g^{\mu\nu} \delta\Gamma^\rho_{\nu\mu} - g^{\mu\rho} \delta\Gamma^\sigma_{\mu\sigma}) = \partial_\rho \sqrt{-g} (g^{\mu\nu} \delta\Gamma^\rho_{\nu\mu} - g^{\mu\rho} \delta\Gamma^\sigma_{\mu\sigma}) \tag{IV.48}$$

which is a total derivative and hence gives, due to Stokes theorem, only a boundary term, which vanishes by definition of $\mathcal{M}$. The remaining terms account to:

$$\delta S_{EH} = \frac{1}{\kappa} \int d^4x \; \delta g^{\mu\nu} \sqrt{-g} \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} \right) \tag{IV.49}$$

which yields the Einstein field equations as extrema. □

IV.B.2 Arnowitt-Deser-Misner Variables

Good references for further details on the Hamiltonian formulation are [50, 244].

Definition IV.B.1 (Spatial metric, shift and lapse function)**.** *Upon splitting $\mathcal{M}$ into a foliation of non-intersecting hypersurfaces $\sigma_t \cong \sigma_{t=0} =: \sigma$, we use the parameter $t \in \mathbb{R}$ as a coordinate and upon choosing a set of spatial coordinates x^a, $a \in \{1, 2, 3\}$, we may express the metric tensor as*

$$g = g_{\mu\nu} \, dx^\mu \otimes dx^\nu =: (-N^2 + q_{ab} N^a N^b) \, dt \otimes dt + 2N^a q_{ab} \, dx^b \otimes dt + q_{ab} \, dx^a \otimes dx^b \tag{IV.50}$$

Here we call $N = N(t, x)$ the lapse function*, $N^a = N^a(t, x)$ the* shift function *and $q_{ab} = q_{ab}(t, x)$ the* spatial *or* intrinsic metric *on σ.*

Due to $\mathcal{M} \cong \mathbb{R} \times \sigma$ there exists a set of diffeomorphism φ_t such that $\sigma_t = \varphi_t(\sigma)$. We define the vector fields

$$T(p) := \frac{\partial\varphi}{\partial t}(t, x) \mid_{\varphi(t,x)=p}, \qquad S_a(p) := \frac{\partial\varphi}{\partial x^a}(t, x) \mid_{\varphi(t,x)=p} \tag{IV.51}$$

Theorem IV.B.2. *Given $(\mathcal{M} \cong \mathbb{R} \times \sigma, g)$ and $(\sigma_t, \varphi_t(\sigma))$ as before. If we split T into a normal and a tangential part (i.e. $n^\mu g_{\mu\nu} S^\nu_a = 0$)*

$$T = N\, n + N^a\, S_a \tag{IV.52}$$

where n is the unit timelike normal of σ_t (i.e. $g_{\mu\nu}(p)n^\mu(p)n^\nu(p) = -1$). Then, we can choose N and N^a as lapse respectively shift fields and

$$q_{ab}(t,x)\mid_{t=0} = (\varphi^* q)_{ab}(t,x) = (S^\mu_a S^\nu_b q_{\mu\nu})(p)\mid_{p=\varphi(t=0,x)}, \qquad q_{\mu\nu} := g_{\mu\nu} + n_\mu n_\nu \tag{IV.53}$$

Proof. First:

$$dx^\mu = \frac{\partial\varphi(t,x)^\mu}{\partial t}dt + \frac{\partial\varphi(t,x)^\mu}{\partial x^a}dx^a = (n^\mu N + N^a S^\mu_a)dt + S^\mu_a dx^a \tag{IV.54}$$

Then using $n_\nu S^\nu_b = 0$ and $n^\mu n_\mu = -1$

$$\begin{aligned} g_{\mu\nu}\, dx^\mu \otimes dx^\nu = g_{\mu\nu} \big[&(n^\mu N^2 n^\nu + N^a N^b S^\mu_a S^\nu_b + 2n^\mu S^\nu_b N^b N)\, dt \otimes dt + \\ &+2(S^\mu_a n^\nu N + N^b S^\mu_a S^\nu_b)\, dx^a \otimes dt + S^\mu_a S^\nu_b\, dx^a \otimes dx^b\big] \\ = (-N^2 + N^a N^b q_{ab})&\, dt \otimes dt + q_{ab} N^b\, dx^a \otimes dt + q_{ab}\, dx^a \otimes dx^b \end{aligned} \tag{IV.55}$$

which was the claim. □

Note also $q_{\mu\nu}n^\mu = n_\nu + (n_\mu n^\mu)n_\nu = 0 = q_{\mu\nu}n^\nu$, a property by which we call $q_{\mu\nu}$ spatial. With $q^\rho_\mu = q_{\mu\nu}g^{\nu\rho}$ follows $q^\rho_\mu = q_{\mu\nu}g^{\nu\rho} = q_{\mu\nu}(q^{\nu\rho} + n^\nu n^\rho) = q_{\mu\nu}q^{\nu\rho}$. Thus, we can use either g or q in order to raise and lower indices of q and indeed of any spatial tensor $t^{\mu_1\cdots\mu_a}_{\nu_1\ldots\nu_b}$, i.e. with $n^{\nu_i} t^{\mu_1\cdots\mu_a}_{\nu_1\ldots\nu_b} = n_{\mu_i} t^{\mu_1\cdots\mu_a}_{\nu_1\ldots\nu_b} = 0$ for all i.
From this follows quickly that

$$\det(\varphi^* g) = -N^2 \det(q_{ab}) \tag{IV.56}$$

Theorem IV.B.3 (Extrinsic curvature)**.** *Given the same structure as before. Consider the* extrinsic curvature *$K_{\mu\nu}$, which is the spatial projection of the parallel transport of the normal n, i.e.*

$$K_{\mu\nu} := q^\rho_\mu q^\sigma_\nu \nabla_\rho n_\sigma \tag{IV.57}$$

Then it holds for $K_{ab}(t,x)\mid_{t=0} := (\varphi^* K)_{ab}(t=0,x)$ that

$$K := q^{\mu\nu}K_{\mu\nu} = q^{ab}K_{ab}, \qquad\qquad K_{ab} = \frac{1}{2N}\left(\dot{q}_{ab} - (\mathcal{L}_{\vec{N}} q)_{ab}\right) \tag{IV.58}$$

Proof. For the first property it suffices to ensure that q^{ab}, the inverse of q_{ab}, fulfils:

$$q^{\mu\nu} = q^{ab} S^\mu_a S^\nu_b \tag{IV.59}$$

For this: $q^{\mu\nu}n_\mu = q^{\mu\nu}n_\nu = 0$ due to $S^\mu_a n_\mu = 0$ as S^μ_a is tangential. As for the spatial-spatial components:

$$(q^{\rho\sigma})q_{\mu\rho}q_{\sigma\nu}S^\mu_a S^\nu_b = q_{\mu\nu}S^\mu_a S^\nu_b = q_{ab} = q^{cd}q_{ac}q_{bd} = (q^{cd}S^\rho_c S^\sigma_d)q_{\mu\rho}q_{\sigma\nu}S^\mu_a S^\nu_b \tag{IV.60}$$

For the second property we notice that

$$(\mathcal{L}_n g)_{\mu\nu} = n^\rho \nabla_\rho g_{\mu\nu} + \nabla_\mu n_\nu + \nabla_\nu n_\mu = 2\nabla_{(\mu}n_{\nu)} \tag{IV.61}$$

which implies

$$K_{\mu\nu} = \frac{1}{2}q^\rho_\mu q^\sigma_\nu (\mathcal{L}_n g)_{\rho\sigma} = \frac{1}{2}\left(q^\rho_\mu q^\sigma_\nu(\mathcal{L}_n q)_{\rho\sigma} + q^\rho_\mu q^\sigma_\nu(\mathcal{L}_n n_\rho n_\sigma)\right) = \frac{1}{2}q^\rho_\mu q^\sigma_\nu(\mathcal{L}_n q)_{\rho\sigma} = \frac{1}{2}(\mathcal{L}_n q)_{\mu\nu} \tag{IV.62}$$

since $q^\sigma_\nu n_\sigma = 0$ and $(\mathcal{L}_n q)_{\rho\sigma}$ being already spatial, since

$$n^\rho(\mathcal{L}_n q)_{\rho\sigma} = n^\rho n^\kappa \partial_\kappa q_{\rho\sigma} + n^\rho(\partial_\rho n^\kappa)q_{\kappa\sigma} + n^\rho(\partial_\sigma n^\kappa)q_{\rho\kappa} = n^\rho\partial_\rho(n^\kappa q_{\kappa\sigma}) = 0 \tag{IV.63}$$

Now we use that $\partial_a T^\mu = \partial_a \partial_0 \varphi^\mu = \partial_0 \partial^\mu_a \varphi = \partial_0 S^\mu_a$ and the chain rule $S^\mu_a \partial_\mu = \partial_a,\ T^\rho\partial_\rho = \partial_t$ for:

$$\begin{aligned} S^\mu_a S^\nu_b(\partial_\mu T^\rho)q_{\nu\rho} &= S^\nu_b(\partial_a T\rho)q_{\nu\rho} = \partial_0(S^\nu_b S^\rho_a q_{\nu\rho}) - S^\rho_a(\partial_0 S^\nu_b)q_{\nu\rho} - S^\rho_a S^\nu_b(\partial_0 q_{\nu\rho}) \\ &= \partial_0 q_{ab} - S^\mu_a S^\nu_b(\partial_0 q_{\mu\nu}) - S^\mu_a(\partial_b T^\rho)q_{\rho\mu} = \dot{q}_{ab} - S^\mu_a S^\nu_b \dot{q}_{\mu\nu} - S^\nu_a S^\mu_b(\partial_\mu T^\rho)q_{\rho\nu} \end{aligned} \tag{IV.64}$$

$$\Rightarrow 2S^\mu_{(a}S^\nu_{b)}(\partial_\mu T^\rho)q_{\nu\rho} = \dot{q}_{ab} - S^\mu_a S^\nu_b \dot{q}_{\nu\mu} \tag{IV.65}$$

which implies

$$S^\mu_a S^\nu_a \mathcal{L}_T q_{\mu\nu} = S^\mu_a S^\nu_b T^\rho \partial_\rho q_{\mu\nu} + 2S^\mu_a S^\nu_b (\partial_{(\mu} T^\rho) q_{\nu)\rho} = S^\mu_a S^\nu_b \partial_0 q_{\mu\nu} + \dot{q}_{ab} - S^\mu_a S^\nu_b \dot{q}_{\nu\mu} = \dot{q}_{ab} \tag{IV.66}$$

Also note that for $S := S_a N^a$ it holds:

$$\begin{aligned} S^\mu_a S^\nu_b (\mathcal{L}_S q)_{\mu\nu} &= S^\mu_c S^\nu_b (S^\rho_c N^c) \partial_\rho q_{\mu\nu} + 2S^\mu_a S^\nu_b q_{\rho(\nu}(\partial_{\mu)} S^\rho_c N^c) \\ &= N^c(\partial_c q_{ab}) - N^c q_{\mu\nu} \partial_c (S^\mu_a S^\nu_b) + 2S^\mu_a S^\nu_b q_{\rho(\nu}((\partial_{\mu)} N^c) S^\rho_c - N^c(\partial_{\mu)} S^\rho_c)) = \\ &= N^c(\partial_c q_{ab}) + 2(\partial_{(a} N^c) q_{b)c} - 2N^c q_{\mu\nu}(\partial_c S^\mu_{(a}) S^\nu_{b)} + 2N^c q_{\rho\nu} S^\nu_{(b} S^\mu_{a)} (\partial_\mu S^\rho_c) = \\ &= \mathcal{L}_{\vec{N}} q_{ab} - 2N^c q_{\mu\nu} S^\nu_{(b} (\partial_{a)} S^\mu_c) + 2N^c q_{\rho\nu} S^\nu_{(b} (\partial_{a)} S^\rho_c) = \mathcal{L}_{\vec{N}} q_{ab} \end{aligned} \tag{IV.67}$$

We can now plug (IV.67) and (IV.66) together into the spatial pull-back of (IV.62) and obtain the wanted result

$$K_{ab} = S^\mu_a S^\nu_b \frac{1}{2N} (\mathcal{L}_T q - \mathcal{L}_S q)_{\mu\nu} = \frac{1}{2N} (\dot{q}_{ab} - (\mathcal{L}_{\vec{N}} q)_{ab}) \tag{IV.68}$$

□

Definition IV.B.2 (Spatial Ricci scalar)**.** *We define the* Ricci scalar *of spatial geometry*[8] *as:*

$$R^{(3)} := -K^2 + K_{\mu\nu} K^{\mu\nu} + q^{\mu\rho} q^{\nu\sigma} R^{(4)}_{\sigma\mu\nu\rho} \tag{IV.69}$$

with $R^{(4)}_{\sigma\mu\nu\rho}$ being the Riemann curvature from (IV.34) for $(\mathcal{M}, g)$.

Lemma IV.B.1 (Codazzi equation)**.** *The relation between the four-dimensional Ricci scalar and spatial Ricci scalar is as follows:*

$$R^{(4)} = R^{(3)} + K_{\mu\nu} K^{\mu\nu} - K^2 - 2\nabla_\mu v^\mu \tag{IV.70}$$

with $v^\mu = n^\nu \nabla_\nu n^\mu - n^\mu \nabla_\nu n^\nu$.

Proof. From its definition (IV.34) follows that $(R^{(4)})^\sigma{}_{\mu\nu\rho} = -(R^{(4)})^\sigma{}_{\nu\mu\rho}$ and we had already seen that $R^{(4)}_{\sigma\mu\nu\rho} = -R^{(4)}_{\rho\mu\nu\sigma}$ in (IV.38). Hence with (IV.36):

$$\begin{aligned} q^{\mu\rho} q^{\nu\sigma} R^{(4)}_{\sigma\mu\nu\rho} &= (g^{\mu\rho} + n^\mu n^\rho)(g^{\nu\sigma} + n^\nu n^\sigma) R^{(4)}_{\sigma\mu\nu\rho} = R^{(4)} + (g^{\mu\rho} n^\nu n^\sigma + g^{\nu\sigma} n^\mu n^\rho) R^{(4)}_{\sigma\mu\nu\rho} = \\ &= R^{(4)} + 2g^{\mu\rho} n^\nu \nabla_{[\mu}, \nabla_{\nu]} n_\rho - 2g^{\nu\sigma} n^\mu \nabla_{[\mu}, \nabla_{\nu]} n_\sigma = \\ &= R^{(4)} + 2\nabla_{[\mu}(n^\nu \nabla_{\nu]} n^\mu - n^\mu \nabla_{\nu]} n^\nu) - ((\nabla_{[\nu} n^\mu)\nabla_{\mu]} n^\nu + (\nabla_{[\mu} n^\mu)\nabla_{\nu]} n^\nu) = \\ &= R^{(4)} + \nabla_\mu (n^\nu \nabla_\nu n^\mu - n^\mu \nabla_\nu n^\nu) \end{aligned} \tag{IV.71}$$

□

Using that $K_{\mu\nu} K^{\mu\nu} = K_{ab} K^{ab}$ under pull-back, (IV.56) and that $\nabla_\mu v^\mu$ is a total derivative and drops out in an integral over $\mathcal{M}$ we can rewrite the Einstein Hilbert action:

$$S_{EH} = \frac{1}{\kappa} \int dt \int d^3x \, N\sqrt{\det(q)} (R^{(3)} + K_{ab} K^{ab} - K^2) \tag{IV.72}$$

One can perform a Legendre transformation of the system to obtain the associated Hamiltonian theory [56]. For this one introduces the following canonical momenta (i.e. $\{q_{ab}, P^{cd}\} = \kappa \delta^c_{(a} \delta^d_{b)} \delta^{(3)}(x,y)$ etc.):

$$\pi := \frac{\delta}{\delta \dot{N}} S_{EH} = 0, \qquad \pi_a := \frac{\delta}{\delta \dot{N}^a} S_{EH} = 0, \qquad P^{ab} := \frac{\delta}{\delta \dot{q}_{ab}} S_{EH} = \frac{1}{\kappa} \sqrt{\det(q)} (K^{ab} - K q^{ab}) \tag{IV.73}$$

Theorem IV.B.4. *Action (IV.72) is equivalent to the Hamiltonian density with Lagrange multipliers v, v^a*

$$H_{GR} = \int_\sigma d^3x \; (\pi v + \pi_a v^a + N^a C_a + NC) \tag{IV.74}$$

where the (spatial) diffeomorphism constraint *C_a and the* scalar constraint *C are given by*

$$C_a := P^{bc} \partial_a q_{bc} - 2\partial_b P^b_a \tag{IV.75}$$

$$C := \frac{\kappa}{\sqrt{\det(q)}} (P^{ab} P_{ab} - \frac{P^2}{2}) - \frac{\sqrt{\det(q)}}{\kappa} R^{(3)} \tag{IV.76}$$

[8] Indeed, it can be shown that this is the usual Ricci scalar (IV.35) of the spatial geometry on σ with a unique covariant differential D compatible with $q_{\mu\nu}$, i.e. $R^{(3)} = R(q) := q^{ab} R^c_{abc}(q)$.

Proof. Note that we can invert P^{ab} by taking the trace: ($q := \det(q)$)

$$P := q_{ab}P^{ab} = -\frac{2}{\kappa}\sqrt{q}K \Rightarrow K^{ab} = \frac{\kappa}{\sqrt{q}}(P^{ab} - q^{ab}\frac{P}{2}) \Rightarrow K^{ab}K_{ab} - K^2 = \frac{\kappa^2}{q}(P_{ab}P^{ab} - \frac{P^2}{2}) \tag{IV.77}$$

With the extremal values $v_{ab} = \dot{q}_{ab} = 2NK_{ab} + (\mathcal{L}_{\vec{N}}q)_{ab}$ follows

$$P^{ab}v_{ab} = 2N\frac{\kappa}{\sqrt{q}}(P_{ab}P^{ab} - \frac{P^2}{2}) + P^{ab}(\mathcal{L}_{\vec{N}}q)_{ab} \tag{IV.78}$$

which implies for the Hamiltonian density

$$\begin{aligned} H_{GR} &= \int_\sigma d^3x \ \left(\pi v + \pi_a v^a + P^{ab}v_{ab} - \mathcal{L}(q_{ab}, N, N^a, v_{ab})\right) = \\ &= \int_\sigma d^3x \left(\pi v + \pi_a v^a + P^{ab}(\mathcal{L}_{\vec{N}}q_{ab}) + N(\frac{\kappa}{\sqrt{q}}(P^{ab}P_{ab} - \frac{P^2}{2} - \frac{\sqrt{q}}{\kappa}R^{(3)})\right) = \\ &= \int_\sigma d^3x \left(\pi v + \pi_a v^a + P^{ab}N^c\nabla_c q_{ab} - 2P^{ab}q_{c(b}\nabla_{a)}N^c + NC\right) \end{aligned} \tag{IV.79}$$

where one can use integration by parts on $P^{ab}q_{c(b}\nabla_{a)}N^c$ in the last line and that the covariant derivative can be replaced with the standard derivative for density weights zero to obtain the claim. □

The name diffeomorphism constraint is indeed justified: By introducing the notion of smeared quantities, e.g. $\vec{C}[\vec{N}] := \int d^3x \ N^a(x)C_a(x)$ one can find that

$$\{\vec{C}[\vec{N}], q_{ab}\} = (\mathcal{L}_{\vec{N}}q)_{ab}, \qquad \{\vec{C}[\vec{N}], P^{ab}\} = (\mathcal{L}_{\vec{N}}P)^{ab} \tag{IV.80}$$

So $\vec{C}[\vec{N}]$ generates diffeomorphisms of σ along the integral curves of $\vec{N}$ on σ.

Lemma IV.B.2 (Hypersurface Deformation Algebra or Dirac Algebra)**.** *The constraint analysis*[9] *of (IV.74) starting with primary constraints $\pi = \pi_a = 0$ yields the* Hypersurface Deformation algebra *as secondary constraints:*

$$\{\vec{C}[\vec{N}], \vec{C}[\vec{N}']\} = -\vec{C}[[\vec{N}, \vec{N}']] \tag{IV.81}$$

$$\{\vec{C}[\vec{N}], C[f]\} = -C[\vec{N}[f]] \tag{IV.82}$$

$$\{C[f], C[g]\} = -\vec{C}[q^{-1}(gdf - fdg)] \tag{IV.83}$$

In other words the complete Hamiltonian density (IV.74) is constrained to vanish[10]*.*

Proof. It is straightforward to see that $0 = \dot{\pi} = \{H, \pi\} = C$ and $0 = \dot{\pi}_a = \{H, \pi_a\} = C^a = 0$ drop out as the secondary constraints. It remains to show that their algebra closes, which is quite technical and, hence, we refer to the literature, e.g. [50]. □

IV.C Connection Formulation of General Relativity

The following subsections address the first steps towards defining a theory for Quantum Gravity. For this we want to follow the Dirac programme introduced in chapter II. However, for the ADM formulation introduced in the last section nobody has succeeded so far in finding (in all generality) a rigorously defined, background independent representation of a suitable quantum algebra which also supports the Hamiltonian constraint operator.

But the situation changed drastically when Ashtekar introduced new canonical variables in 1986-88. Hence, in this section we follow his strategy to rewrite GR in the connection formulation and introduce a possible candidate for an algebra of observables, i.e. the holonomy-flux algebra.

[9] This physical procedure to treat singular Lagrangians was originally worked out by Dirac: If a function f is constrained to vanish for a system at *all* times, it follows that also its time derivative has to vanish, $\dot{f} = \{H, f\} = 0$. However this condition may yield a further (so-called) secondary constraints, for which the same argument must apply. The whole set of conditions obtained by this iterative procedure is called the *constraint algebra*.

[10] This is known as the *problem of time* in GR. It comes about as the Hamiltonian density H only generates gauge transformations and not an observable time evolution. A way out of the situation is to couple GR to some matter fields, which can serve as clocks [147–153]. This yields a physical Hamiltonian which is in general different from H. We will come back to this strategy in section IV.D where we will use a massless scalar field (IV.208) as reference frame.

IV.C.1 Derivation of the Ashtekar-Barbero Variables

With the intent of ultimately defining a theory of Quantum Gravity, major developments were made when reformulating GR in terms of a gauge theory of Yang-Mills type. Originally motivated by the discoveries of Sen [57–59], this was achieved first by Ashtekar [53–55] and later improved by Barbero [60, 61] by making explicit use of $\dim \mathcal{M} = 4$ as will be reviewed in the following.

Definition IV.C.1 (3-bein & co-3-bein). *One defines the* co-3-bein *fields* e_a^I *on* σ *(with spacetime indices* a *and internal indices* $I = 1, .., 3$*) such that*

$$q_{ab} = \delta_{IJ} e_a^I e_b^J \tag{IV.84}$$

Note that tensorial indices are pulled via q_{ab} *while we define internal ones to be raised and lowered with* δ_{IJ}*. Since also* q_{ab} *is by definition invertible there exists an inverse, called* 3-bein e_I^a*, such that*

$$e_I^a e_b^I := \delta_{IJ} e^{Ia} e_b^J = q^{ab} q_{bc} = \delta_b^a, \qquad e_a^I e_J^a = e_I^a q_{ab} e_J^b = e_I^a e_a^K \delta_{KL} e_b^L e_J^b = \delta_{IJ} \tag{IV.85}$$

This will always be possible as one can see by counting the degrees of freedom: q_{ab} has 6 (due to being symmetric), while e_a^I has 9 dof. This reflects that we have introduced some gauge degrees of freedom, as q_{ab} is invariant under local SO(3) rotations $e_a^I \mapsto O_J^I(x) e_a^J$ since $\delta_{IJ} O_K^I(x) O_L^J(x) = \delta_{KL}$.

Definition IV.C.2 (Spin connection). *Let* D *be the unique covariant derivative which is compatible with the spatial metric* q_{ab}*, i.e.* $Dq = 0$*. We define its extension acting on generalised tensors with additional internal indices by*

$$D_a t^{a_1..a_n}_{b_1..b_m\ J_1..J_p} := (D_a t^{a_1..a_n}_{b_1..b_m})_{J_1..J_p} \quad + \sum_{i=1}^{p} \Gamma_a^M \epsilon_{J_i ML} \quad t^{a_1..a_n}_{b_1..b_m\ J_1..\not{J}_i L..J_p} \tag{IV.86}$$

where the spin connection Γ *is given by*

$$\Gamma_a^L := -\frac{1}{2}\epsilon^{LJK} e_K^b \left(\partial_b e_a^J - \partial_a e_b^J + e_J^c e_a^M \partial_b e_c^M\right) \tag{IV.87}$$

Lemma IV.C.1. *For the spin connection defined in (IV.87) holds*

$$D_a e_b^J = 0 \tag{IV.88}$$

Proof. Assuming $D_e e_J^a = 0$ we determine the structure of $\Gamma_{eJK} := \Gamma_e^L \epsilon_{JLK}$. First note that $\Gamma_{e(JK)} = 0$ since

$$2\Gamma_{e(JK)} = \partial_e \delta_{IJ} + \Gamma_{eJ}^{\ \ L} \delta_{LK} + \Gamma_{eK}^{\ \ L} \delta_{JL} = D_e \delta_{JK} = D_e(e_J^a e_K^b q_{ab}) = 0 \tag{IV.89}$$

Also note for the connection associated with D, i.e. $\Gamma_{abc} = \frac{1}{2}(\partial_b q_{ac} + \partial_a q_{bc} - \partial_c q_{ab})$ that

$$D_{[a} e_{b]}^J = 0 = \partial_{[a} e_{b]}^J + \Gamma_{[aJK} e_{b]}^K - \Gamma_{[ab]}^c e_c^J = \partial_{[a} e_{b]}^J + \Gamma_{[aJK} e_{b]}^K \tag{IV.90}$$

By defining $\gamma_{JKL} := 2 e_{[K}^a e_{L]}^b \partial_a e_{bJ}$ and $\Gamma_{KJL} := e_K^a \Gamma_{aJL}$, it can be rewritten:

$$0 = \gamma_{JKL} + \Gamma_{KJL} - \Gamma_{LJK} = 2 e_K^a e_L^b \left(\partial_{[a} e_{b]}^J + \Gamma_{aJL'} e_b^{L'} - \Gamma_{bJK'} e_a^{K'}\right) \tag{IV.91}$$

Using $\Gamma_{e(JK)} = 0$ gives

$$2\Gamma_{KJL} = (\Gamma_{KJL} - \Gamma_{LJK}) + (\Gamma_{JLK} - \Gamma_{KLJ}) - (\Gamma_{LKJ} - \Gamma_{JKL}) = -(\gamma_{JKL} + \gamma_{LJK} - \gamma_{KLJ}) \tag{IV.92}$$

Upon plugging together:

$$\begin{aligned}
-\Gamma_a^L &= \frac{1}{2}\epsilon^{LJK}\Gamma_{aJK} = \frac{1}{2}\epsilon^{LJK}(e_a^M \Gamma_{MJK}) = -\frac{1}{4}\epsilon^{LJK} e_a^M (\gamma_{JMK} + \gamma_{KJM} - \gamma_{MKJ}) = \\
&= \frac{e_a^M}{4}\epsilon^{LJK}(2\gamma_{JKM} - \gamma_{MJK}) = \frac{e_a^M}{4}\epsilon^{LJK}(4 e_{[K}^b e_{M]}^c \partial_b e_{cJ} - 2 e_{[J}^b e_{K]}^c \partial_b e_{cM}) = \\
&= -\frac{e_K^b}{2}\epsilon^{LJK}(2\partial_{[a} e_{b]J} - e_J^c e_a^M \partial_b e_c^M)
\end{aligned} \tag{IV.93}$$

□

Definition IV.C.3 (Ashtekar-Barbero variables)**.** *The* Ashtekar-Barbero variables *coordinatise the phase space of an* SU(2) *Yang-Mills theory, described by an* SU(2) *connection (gauge potential)* $A_a^J := \epsilon^{JKL} A_a^{(KL)}/2$ *and a non-abelian electric field* E_J^a*, which satisfy the algebra:*

$$\{E_J^a(x), E_K^b(y)\} = 0 \tag{IV.94}$$

$$\{A_a^J(x), A_b^K(y)\} = 0 \tag{IV.95}$$

$$\{E_J^a(x), A_b^K(y)\} = \frac{\kappa\beta}{2} \delta_b^a \delta_K^J \delta^{(3)}(x, y) \tag{IV.96}$$

with $\beta \in \mathbb{R} - \{0\}$*, the so-called* Immirzi parameter*. This phase space is subject to the Gauss constraint:*

$$G_J = \mathcal{D}_a E_J^a = \partial_a E_J^a + \epsilon_{JKL} A_a^K E_L^a = 0 \tag{IV.97}$$

Theorem IV.C.1 (Ashtekar, Barbero, Sen, Immirzi, 1986-94)**.** *The phase space of the Ashtekar-Barbero variables becomes identical with the phase space of the ADM framework of GR under the identification:*

$$A_a^J := \Gamma_a^J + \beta K_{ab} e_J^b, \qquad E_J^a :=\mid \det(e) \mid e_J^a, \qquad (\epsilon^{abc} e_a^J = \frac{sgn(\det(e))}{\sqrt{\det(q)}} \epsilon^{JKL} E_K^a E_L^b) \tag{IV.98}$$

with $\det(e) := \det(\{e_a^I\}_a^I)$*. This results in*

$$\mathbb{Q}^{ab}(A, E) := \delta^{JK} E_J^a E_K^b \frac{1}{\mid \det(E) \mid}, \qquad \mathbb{P}^{ab}(A, E) := \frac{1}{\beta\kappa} (\mathbb{Q}^{c(a}\mathbb{Q}^{b)d} - \mathbb{Q}^{ab}\mathbb{Q}^{cd})(A_c^J - \Gamma_c^J)\mathbb{Q}_{de} E_J^e \tag{IV.99}$$

having the same Poisson brackets as P^{ab}, q_{ab} *as long as the Gauss constraint* $G_J = 0$ *holds.*

The astonishing fact is, that this works only in $D = 3$ dimension: the connection is valued in the Lie algebra of $\mathrm{SU}(2) \cong \mathrm{so}(3)$ which has dimension $\frac{1}{2}D(D-1) = D$. Thus, one has as many A-fields as E.

Proof. Notice that $\det(E) = \det(e^{-1}) \mid \det(e) \mid^3 = \pm \mid \det(e) \mid^2 \Rightarrow \mid \det(E) \mid = \det(q)$, which can be easily checked if written as ϵ-contractions. Hence

$$\mathbb{Q}^{ab} = \frac{\mid \det(e) \mid^2}{\det(q)} e_J^a e_K^b \delta^{JK} = q^{ab} \Rightarrow \{\mathbb{Q}_{ab}(x), \mathbb{Q}_{cd}(y)\} = 0 \tag{IV.100}$$

In an intermediate step note that

$$\epsilon_{abc} E_I^a E_J^b E_K^c = \det(E) \epsilon_{IJK}, \qquad \epsilon^{IJK} E_I^a E_J^b E_k^c = \det(E) \epsilon_{abc} \tag{IV.101}$$

as either $I = J$ and similar imply $0 = 0$ and $\{IJK\} = \sigma\{123\}$ implies $\epsilon^{abc} E_a^I E_b^j E_c^K = \epsilon^{abc} E_a^1 E_b^2 E_c^3 \times sgn(\sigma\{IJK\}) = \det(E)\epsilon_{IJK}$. The same argument holds of course also for exchanging spacetime and internal indices. From here one deduces that

$$e_a^J \epsilon^{abc} = \frac{\mid \det(e) \mid}{\det(E)} \epsilon^{JKL} E_K^b E_L^c = \frac{sgn(\det(e))}{\sqrt{\det(q)}} \epsilon^{JKL} E_K^b E_L^c \tag{IV.102}$$

as was claimed in (IV.98) and furthermore

$$\begin{aligned} \{A_d^J, \det(E)\} &= \frac{1}{2} \epsilon^{ILK} E_I^a E_L^b \{A_d^J, E_K^c\} \epsilon_{abc} = -\frac{\kappa\beta}{4} \epsilon^{ILJ} \epsilon_{abd} E_I^a E_L^b = -\frac{\kappa\beta}{4} \epsilon_{abd} \epsilon^{fab} e_f^J \frac{\sqrt{\det(q)}}{sgn(\det(e))} = \\ &= -\frac{\kappa\beta}{2} \det(e) e_d^J =: -\frac{\kappa\beta}{2} \det(E) E_d^J \end{aligned} \tag{IV.103}$$

With this and $\Gamma_a^J = \Gamma_a^J(e) \mid_{E_J^a = \mid\det(e)\mid e_J^a}$ one evaluates

$$\begin{aligned} \{\mathbb{P}^{ab}(x), \mathbb{Q}_{ef}(y)\} &= \frac{1}{\beta\kappa} (\mathbb{Q}^{c(a}\mathbb{Q}^{b)d} - \mathbb{Q}^{ab}\mathbb{Q}^{cd})\mathbb{Q}_{dg} E_J^g)(x) \{A_c^J(x), \mathbb{Q}_{ef}(y)\} = \\ &= \frac{1}{\beta\kappa} (\mathbb{Q}^{c(a}\mathbb{Q}^{b)d} - \mathbb{Q}^{ab}\mathbb{Q}^{cd})\mathbb{Q}_{dg} E_J^g)(x) \mathbb{Q}_{em}(y) \{A_c^J(x), \mathbb{Q}^{mn}(y)\} \mathbb{Q}_{nf}(y) = \\ &= \frac{1}{2} (\mathbb{Q}^{c(a}\mathbb{Q}^{b)d} - \mathbb{Q}^{ab}\mathbb{Q}^{cd}) \mathbb{Q}_{em}\mathbb{Q}_{nf}\mathbb{Q}_{dg} (\delta_c^m \mathbb{Q}^{gn} + \mathbb{Q}^{mg}\delta_c^n - \frac{1}{2}\mathbb{Q}^{mn}\delta_c^g)(x) \delta^{(3)}(x, y) = \\ &= \frac{1}{2} (\mathbb{Q}^{c(a}\mathbb{Q}^{b)d} - \mathbb{Q}^{ab}\mathbb{Q}^{cd})(\mathbb{Q}_{e(c}\mathbb{Q}_{d)f} - \frac{1}{2}\mathbb{Q}_{ef}\mathbb{Q}_{dc})(x) \delta^{(3)}(x, y) = \delta_e^a \delta_f^b \delta^{(3)}(x, y) \end{aligned} \tag{IV.104}$$

Prior to the last bracket let us state that

$$\frac{\delta}{\delta E^b_J}F(E) := \frac{\delta}{\delta E^b_J}\int d^3x\, \Gamma^L_b E^b_J = \Gamma^J_b \tag{IV.105}$$

since ($e := \det(e)$)

$$\begin{aligned}
E^a_L\delta\Gamma^L_a &= \frac{1}{2}\mid e\mid \epsilon^{LJK}\left(\delta(2e^b_{[K}e^a_{L]}\partial_b e^J_a + e^b_K e^a_J \partial_b e^L_a) - (\delta e^a_L)e^b_K(2\partial_{[b}e^J_{a]} + e^c_J e^b_K e^M_a \partial_b e^M_c)\right) = \\
&= \frac{1}{2}\mid e\mid \epsilon^{LJK}\left(\delta(e^b_K e^a_L)\partial_b e^J_a + e^b_K e^a_L \partial_b \delta e^J_a - 2(\delta e^{[a}_L)e^{b]}_K \partial_b e^J_a - (\delta e^a_L)e^M_a e^b_K e^C_J \partial_b e^M_c\right) = \\
&= \frac{1}{2}\mid e\mid \epsilon^{JKL}\left(e^b_K e^a_L \delta\partial_b e^J_a - \delta(e^a_L e^M_a)e^b_K e^c_J \partial_b e^M_c + (\delta e^M_a)\partial_b e^M_c e^b_K e^c_J\right) = \\
&= \frac{1}{2}\left(\epsilon^{cba}e^J_c\delta\partial_b e^J_a + \epsilon^{cbd}e^L_d e^a_L(\partial_b e^M_c)(\delta e^M_a)\right) = \\
&= \frac{\epsilon^{abc}}{2}(-e^J_c\partial_b\delta e^J_a - (\partial_b e^M_c)\delta e^M_a) = -\frac{\epsilon^{abc}}{2}\partial_b(e^J_c\delta E^J_a) = d(e^J\wedge\delta e_J)
\end{aligned} \tag{IV.106}$$

where we have used again a version of (IV.101) to obtain the fourth line. But by being a total derivative the term drops in the integral yielding (IV.105).
Finally the third bracket:

$$\begin{aligned}
\{\mathbb{P}^{ab}(x),\mathbb{P}^{cd}(y)\}(\beta\kappa)^2 &= (\mathbb{Q}^{e(a}E^{b)}_J - \mathbb{Q}^{ab}E^e_J)(x)(A^K_f - \Gamma^K_f)(y)\{A^J_e(x),(\mathbb{Q}^{f(c}E^{d)}_K - \mathbb{Q}^{cd}E^f_K)(y)\} - \\
&- (\mathbb{Q}^{f(c}E^{d)}_K - \mathbb{Q}^{cd}E^f_K)(y)(A^J_e - \Gamma^J_e)(x)\{A^K_f(y),(\mathbb{Q}^{e(a}E^{b)}_J - \mathbb{Q}^{ab}E^e_J)(x)\} + \\
&+ (\mathbb{Q}^{e(a}E^{b)}_J - \mathbb{Q}^{ab}E^e_J)(x)(\mathbb{Q}^{f(c}E^{d)}_K - \mathbb{Q}^{cd}E^f_K)(y)\{A^J_e - \Gamma^J_e)(x),(A^K_f - \Gamma^K_f)(y)\}
\end{aligned} \tag{IV.107}$$

where the last bracket is found to vanish due to (IV.105):

$$\begin{aligned}
\{(A^J_e - \Gamma^J_e)(x),(A^K_f - \Gamma^K_f)(y)\} &= \{A^J_e(x),A^K_f(y)\} + \{A^J_e(x),\Gamma^K_f(y)\} - \{\Gamma^J_e(x),A^K_f(y)\} + \{\Gamma^J_e,\Gamma^K_f\} = \\
&= \frac{\beta\kappa}{2}\left(\frac{\delta\Gamma^K_f(y)}{\delta E^e_J(x)} - \frac{\delta\Gamma^J_e(x)}{\delta E^f_K(y)}\right) = \frac{\beta\kappa}{2}\left(\frac{\delta^2}{\Delta E^e_J(x)\delta E^f_K(y)} - \frac{\delta^2}{\delta E^f_K(y)\delta E^e_J(x)}\right)F(E) = \\
&= 0
\end{aligned} \tag{IV.108}$$

After some calculation one finds

$$\{\mathbb{P}^{ab}(x),\mathbb{P}^{cd}(y)\} = \frac{\delta(x,y)}{4\beta\kappa}(\mathbb{Q}^{ac}G^{[bd]} - \mathbb{Q}^{ad}G^{[bc]} + \mathbb{Q}^{bc}G^{[da]} - \mathbb{Q}^{bd}G^{[ac]}) \tag{IV.109}$$

with (using IV.102)

$$G^{[ab]} = E^c_J E^{[a}_J E^{b]}_K(A^K_c - \Gamma^K_c)\frac{1}{\det(E)} = \epsilon^{abd}E^L_d\epsilon_{LJK}(A^J_c - \Gamma^J_c)E^c_K \tag{IV.110}$$

However, since $D_a e^J_b = 0 \Rightarrow D_a e^b_J = 0 \Rightarrow D_a E^b_J = 0$ it follows

$$D_a E^a_J = \partial_a E^a_J + \Gamma^L_a\epsilon_{JLK}E^a_K = 0 \Rightarrow \epsilon_{LJK}(A^J_c - \Gamma^J_c)E^c_K = \partial_c E^c_J + \epsilon_{JLK}A^L_a E^a_K = G_J \tag{IV.111}$$

In other words $G^{[ab]}$ (and thus (IV.109)) is zero if the Gauss law (IV.97) holds, which was the claim. □

Theorem IV.C.2. *The Hamiltonian density of GR, given by (IV.75) and (IV.76), can be rewritten in terms of the Ashtekar-Barbero variables as*

$$C_a = \frac{2}{\kappa\beta}F^J_{ab}(A)E^b_J \tag{IV.112}$$

$$C := \frac{4}{\kappa^2\beta}\left(F^J_{ab}(A) - \frac{1+\beta^2}{\beta^6}\frac{4}{\kappa^2}\epsilon_{JMN}\{\{V,C_E[1]\},A^M_a\}\{\{V,C_E[1]\},A^N_b\}\right)\epsilon^{abc}\{V,A^J_c\} \tag{IV.113}$$

where the spatial volume V*, the* curvature of the Ashtekar connection $F^J_{ab}(A)$ *and the* Euclidian part of the scalar constraint*,* C_E*, are explicitly*

$$V := \int_\sigma d^3x\,\sqrt{\mid\det(E)\mid} \tag{IV.114}$$

$$F^J_{ab}(A) := 2\partial_{[a}A^J_{b]} + \epsilon^J{}_{KL}A^K_a A^L_b \tag{IV.115}$$

$$C_E := \frac{4}{\kappa^2\beta}sgn(\det(e))F^J_{ab}\epsilon^{abc}\{V,A^J_c\} = \frac{1}{\kappa}F^J_{ab}\epsilon_{JKL}\frac{E^a_K E^b_L}{\sqrt{\det(q)}} \tag{IV.116}$$

This theorem bears significant importance for the (later discussed) purpose of developing a quantum theory of gravity: It allows to express the physical constraints without the problematic factor $1/\det(q)$. We will later see that this is the key for a rigorous quantisation of the Hamiltonian of GR in Ashtekar-Barbero variables in the way originally intended by Dirac.
For the proof of the theorem we need first the following Lemma due to Thiemann [74, 75].

Lemma IV.C.2 (Thiemann identities)**.** *It holds*

$$\{V, A_a^J\} = \frac{\kappa\beta}{8} sgn(\det(e))\epsilon^{JKL}\epsilon_{abc}\frac{E_K^b E_L^c}{\sqrt{|\det(E)|}} \tag{IV.117}$$

$$\{\{V, C_E[1]\}, A_a^J\} = \frac{\kappa\beta^3}{2} sgn(\det(e))K_{ab}e_J^b \tag{IV.118}$$

Proof. We already computed in (IV.103) that $\{A_d^J, \det(E)\} = -\frac{\kappa}{2}\det(e)e_d^J$. Thus follows with (IV.102) that

$$\frac{\delta V}{\delta E_J^a} = \frac{1}{2}e_a^J = \frac{1}{4} sgn(\det(e))\epsilon^{JKL}\epsilon_{abc}\frac{E_K^b E_L^c}{\sqrt{\det(q)}} \tag{IV.119}$$

which is the first claim. Also with $C_E[1] = sgn(\det(e))/(\kappa)\int_\sigma d^3x F_{ab}^I\epsilon^{abc}e_c^L\delta_{IL}$ we compute

$$\begin{aligned}
sgn(\det(e))\frac{\delta C_E[1]}{\delta A_d^J(x)} &= -\frac{2}{\kappa}\delta_{[b}^d\epsilon^{abc}\partial_{a]}e_c^L\delta_{JL} + \frac{2}{\kappa}\epsilon_{IKM}\delta_M^J A_a^K\epsilon^{adc}e_c^L\delta_{IL} = -\frac{2}{\kappa}\epsilon^{adc}(\epsilon_{JKL}A_a^K e_c^L + \partial_a e_c^J) = \\
&= -\frac{2}{\kappa}\epsilon^{adc}(A_a^K\epsilon_{JKL}e_c^L - \Gamma_a^K\epsilon_{JKL}e_c^L + \partial_a e_c^J + \Gamma_a^K\epsilon_{JKL}e_c^L) = \\
&= -\frac{2}{\kappa}\epsilon^{adc}(\beta K_{ab}e_K^b\epsilon_{JKL}e_c^L + D_a E_c^J) = -\frac{2}{\kappa}\epsilon^{adc}\beta K_{ab}e_K^b\epsilon_{JKL}e_c^L
\end{aligned} \tag{IV.120}$$

From both follows:

$$\begin{aligned}
K :&= \{V, C_E[1]\} = \frac{\beta\kappa}{2}\int_\sigma d^3x\ \frac{\delta V}{\delta E_J^d(x)}\frac{\delta C_E[1]}{\delta A_d^J(x)} = -\beta^2/2 sgn(\det(e))\int_\sigma d^3x\ e_d^J K_{ab}e_K^b(e_K^f e_f^M)\epsilon_{JML}e_c^L\epsilon^{adc} = \\
&= \beta^2 sgn(\det(e))\int_\sigma d^3x\ K_{ab}e_K^b e_K^f\det(e)\delta_f^a = \beta^2 sgn(\det(e))\int_\sigma d^3x\ K_{ab}e_K^b E_K^a
\end{aligned} \tag{IV.121}$$

Now one can easily see with (IV.105) that

$$\begin{aligned}
sgn(\det(e))\{K, A_d^J\} &= \frac{\beta\kappa}{2}\beta^2\frac{\delta}{\delta E_J^a(x)}\int_\sigma d^3y\ K_{ab}e_K^b E_K^a = \frac{\beta^3\kappa}{2}\frac{\delta}{\delta E_J^d(x)}(\int d^3x(A_a^K E_K^a - F[E]) \\
&= \frac{\beta^3\kappa}{2}(A_a^J - \Gamma_a^J) = \frac{\beta^3\kappa}{2}K_{ab}e_J^b
\end{aligned} \tag{IV.122}$$

which finishes the Lemma. □

Proof of theorem IV.C.2. Before looking at the expression which will turn out to be the diffeomorphism constraint in Ashtekar-Barbero variables, let us look at the following equation (for any vector field v):

$$\begin{aligned}
D_{[a}D_{b]}v_c^J &= D_{[a}(\Gamma_{b]}^M\epsilon_{JMK}v_c^K + (D_{b]}v_c)^J) = \qquad \text{(IV.123)} \\
&= (D_{[a}D_{b]}v_c)^J + \epsilon_{JMK}(\Gamma_{[a}^M(D_{b]}v_c)^K - \Gamma_{[b}^M(D_{a]}v_c)^K + (\partial_{[a}\Gamma_{b]}^M)v_c^K - \Gamma_{[b}^M\Gamma_{a]}^N\epsilon_{KNL}v_c^L) = \\
&= (D_{[a}, D_{b]}v_c)^J + (\partial_{[a}\Gamma_{b]}^M)\epsilon_{JML}v_c^L + \Gamma_b^M\Gamma_a^N\epsilon_{KJ[M}\epsilon_{N]LK}v_c^L = \\
&= R_{dabc}(q)q^{de}v_e^J + ((\partial_{[a}\Gamma_{b]}^M) + \Gamma_b^M\Gamma_a^N\epsilon_{KNM}\frac{1}{2})\epsilon_{JML}v_c^L =: R^d{}_{abc}(q)v_d^J + \frac{1}{2}F_{ab}^K(\Gamma)\epsilon_{JKL}v_c^L
\end{aligned}$$

where we defined $F_{ab}^K(\Gamma)$, the curvature of the spin-connection. As the left hand vanishes for $v_c^J = e_c^J$ this leads to

$$F_{ab}^J(\Gamma)E_J^b = \frac{1}{2}\epsilon_{LKJ}E_J^b e_L^c e_K^d R_{dabc}(q) = \det(e)/2\epsilon^{bcd}R_{dabc}(q) = -\frac{\det(e)}{2}\epsilon^{bcd}R_{a[bcd]} = 0 \tag{IV.124}$$

since for all one-forms ω:

$$0 = (d^2\omega)_{bcd} = 2\nabla_{[b}\nabla_c\omega_{d]} = \nabla_{[b}\nabla_c\omega_{d]} - \nabla_{[c}\nabla_b\omega_{d]} = R^a{}_{[bcd]}\omega_a \tag{IV.125}$$

The curvature of the spin connection is related to the curvature $F^J_{ab} = F^J_{ab}(A)$ by

$$F^J_{ab} = 2\partial_{[a}A^J_{b]} + \epsilon_{JKL}A^K_a A^L_b = F^J_{ab}(\Gamma) + 2\beta D_{[a}K^J_{b]} + \beta^2\epsilon_{JKL}K^K_a K^L_b \tag{IV.126}$$

such that in the following contraction we can use (IV.124) for the first term:

$$\begin{aligned}F^J_{ab}(A)E^b_J &= F^J_{ab}(\Gamma)E^b_J + \beta(D_aK_{bc}e^c_J E^b_J - D_bK_{ac}e^c_J E^b_J) + \beta^2\epsilon_{JKL}K_{ac}e^c_K K_{bd}e^d_L E^b_J = \\ &= -\beta\sqrt{\det(q)}D_b(K^b_a - q^b_a K) + \beta^2\sqrt{\det(q)}\det(e)\epsilon^{cdb}K_{ac}K_{bd} = \\ &= -\beta\kappa D_b P^b_a\end{aligned} \tag{IV.127}$$

where we have used $K_{[bd]} = 0$ for the last line. Finally we obtain (IV.112) when removing the density weight due to metric compatibility ($q := \det(q)$, $P^b_a =: \sqrt{\det(q)}p^b_a$)

$$\begin{aligned}D_bP^b_a &= D_b(\sqrt{\det(q)}p^b_a) = \sqrt{q}D_bp^b_a = \sqrt{q}(\partial_bp^b_a + \Gamma^b_{bc}p^c_a - \Gamma^c_{ba}p^b_c) = \\ &= \sqrt{q}\left(\partial_cp^c_a + \frac{1}{2}p^c_a q^{be}\partial_e q_{bc} + \frac{1}{2}p^c_a q^{be}\partial_{[c}q_{b]e} - \frac{1}{2}p^b_c q^{ce}\partial_e q_{ba} - \frac{1}{2}p^{be}\partial_{[a}q_{b]e}\right) = \\ &= \partial_c(\sqrt{q}p^c_a) + \frac{1}{2}P^c_a q^{be}(\partial_e q_{bc} - \partial_b q_{ce}) - \frac{1}{2}P^{be}\partial_a q_{be} - \frac{1}{2}P^{be}(\partial_e q_{ba} - \partial_b q_{ae}) = \\ &= \partial_c P^c_a - \frac{1}{2}P^{ce}\partial_a q_{be} = -\frac{1}{2}C_a\end{aligned} \tag{IV.128}$$

For the scalar constraint we first rewrite part of $C_E = \frac{1}{\kappa}sgn(\det(e))F^I_{ab}\epsilon_{JKL}\frac{E^a_K E^b_L}{\sqrt{\det(q)}}$, namely

$$\begin{aligned}F^J_{ab}(A)\epsilon_{JKL}E^a_K E^b_L &= (F^J_{ab}(\Gamma)E^a_K E^b_L + 2\beta D_{[a}K_{b]c}e^c_J E^a_K E^b_L + \beta^2\epsilon_{JMN}K_{ac}e^c_M K_{bd}e^d_N E^a_K E^b_L)\epsilon_{JKL} = \\ &= R_{dabc}(q)e^c_K e^d_L E^a_L E^b_K + 2\beta D_a K_{bc}\epsilon^{cba}\det(E) - \beta^2(K_{ab}K^{ab} - K^2)\mid\det(E)\mid \\ &= (-R_{bd}(q)q^{bd} - \beta^2(K_{ab}K^{ab} - K^2))\mid\det(E)\mid\end{aligned} \tag{IV.129}$$

which tells us that $s := sgn(\det(e))$

$$\begin{aligned}C &= \sqrt{\det(q)}/\kappa(K_{ab}K^{ab} - K^2 - R^{(3)}(q)) = C_E + \frac{1+\beta^2}{\kappa}\sqrt{\det(q)}(K_{ab}K^{ab} - K^2) = \\ &= C_E - s\frac{1+\beta^2}{\kappa}K_{ac}e^c_M K_{bd}e^d_N\epsilon_{MNJ}\epsilon^{JKL}\frac{E^a_K E^b_L}{\sqrt{\det(E)}} = \\ &= s\frac{4}{\kappa^2\beta}\left(F^J_{ab} - \frac{1+\beta^2}{\kappa^2\beta^6}4\{K, A^M_a\}\{K, A^N_b\}\epsilon_{MNJ}\right)\epsilon^{abc}\{V, A^J_c\}\end{aligned} \tag{IV.130}$$

Lastly, we substitute the lapse function $N \to sgn(\det(e))N$ and obtain the claim. □

IV.C.2 The Holonomy-flux algebra

By introducing the new SU(2)-phase space variables (A^I_a, E^b_J) one also introduced a new constraint into the framework of GR, namely the Gauss constraint G_J from (IV.97). Thus, we have to complete the constraint analysis with respect to it and ensure that no new conditions arise from the Poisson brackets with $C[N]$ and $\vec{C}[\vec{N}]$.
For this purpose we will express the constraint in terms of smearings of the fundamental variables, connection $A^I_a(x)$ and electric field $E^a_I(x)$. Smearing can be done in general e.g. with any test function, however to ensure a nice behaviour under gauge transformations it will turn out to be useful to smear along distributional objects, i.e. curves and surfaces.
We will make all of this precise in the following. References covering further details and including the theorems mentioned below are for example [48, 50].

Definition IV.C.4 (Pauli matrices)**.** *Consider a basis of the Lie-algebra* $\mathfrak{su}(2)$*, namely* $\tau_I := -i\sigma_I/2$ *where* σ_I *are the* Pauli matrices[11]*. Explicitly the* τ_I *are given by* $(I = 1, 2, 3)$

$$\tau_1 := -\frac{1}{2}\begin{pmatrix} 0 & i \\ i & 0\end{pmatrix}, \qquad \tau_2 := -\frac{1}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}, \qquad \tau_3 := -\frac{1}{2}\begin{pmatrix} i & 0 \\ 0 & -i\end{pmatrix} \tag{IV.131}$$

[11] By this choice of basis one identifies the structure function of $\mathfrak{su}(2)$ with ϵ_{IJK}, the Levi-Civita symbol as is appearing e.g. in (IV.97).

which indeed are satisfying the algebraic relation of $\mathfrak{su}(2)$*, i.e.*

$$[\tau_I, \tau_J] = \epsilon_{IJK}\tau_K \tag{IV.132}$$

Lemma IV.C.3 (Infinitesimal gauge transformations)**.** *The infinitesimal smeared Gauss constraint* ($\Lambda^J \in \mathcal{S}$)

$$G(\Lambda) := \int_\sigma d^3x\ \Lambda^J G_J = -\int_\sigma d^3x\ E^a_J(\partial_a\Lambda^J + \epsilon_{JKL}A^K_a\Lambda^L) \tag{IV.133}$$

produces the following infinitesimal transformations:

$$\{G(\Lambda), A_a\} = \frac{\beta\kappa}{2}(-\partial_a\Lambda + [\Lambda, A_a]) \tag{IV.134}$$

$$\{G(\Lambda), E^a\} = \frac{\beta\kappa}{2}[\Lambda, E^a] \tag{IV.135}$$

$$\{G(\Lambda), G(\Lambda')\} = -\frac{\beta\kappa}{2}G([\Lambda, \Lambda']) \tag{IV.136}$$

with $A_a := A^J_a\tau_J$*,* $E^a := E^a_J\tau_J$ *and* $\Lambda := \Lambda^J\tau_J$*.*

Proof. With $\delta A_a(x)/\delta A^I_b(y) = \tau_I\delta^b_c\delta(x,y)$ follow the first two relations immediately from

$$\frac{\delta G(\Lambda)}{\delta E^b_I} = -(\partial_b\Lambda^I + \epsilon_{IKL}A^K_b\Lambda^L), \qquad \frac{\delta G(\Lambda)}{\delta A^I_b} = -E^b_J\epsilon_{JIL}\Lambda^L \tag{IV.137}$$

and since $[\Lambda, \Lambda']^I = \epsilon_{IJK}\Lambda^J\Lambda'^K$:

$$\begin{aligned}
\{G([\Lambda]), G[\Lambda']\} &= (-\frac{\beta\kappa}{2})(-\epsilon_{ILJ}\Lambda^L E^b_J)(-\partial_b\Lambda'^I + \epsilon_{IKM}\Lambda'^K A^M_b) - (\Lambda \leftrightarrow \Lambda') = \\
&= -\frac{\beta\kappa}{2}\left(\epsilon_{ILJ}E^b_J\partial_b\Lambda^L\Lambda'^I + \epsilon_{ILJ}\epsilon_{IKM}(\Lambda^L\Lambda'^K - \Lambda'^L\Lambda^K)E^b_J A^M_b\right) = \\
&= -\frac{\beta\kappa}{2}E^b_J\left(\partial_b(\epsilon_{ILJ}\Lambda^L\Lambda'^I) - 2\Lambda^{[M}\Lambda'^{J]}A^M_b\right) = \\
&= -\frac{\beta\kappa}{2}E^b_J\left(\partial_b[\Lambda, \Lambda']^J + \epsilon_{JKL}(\epsilon^{LJ'K'}\Lambda^{J'}\Lambda'^{K'})A^K_b\right) = -\frac{\beta\kappa}{2}G([\Lambda, \Lambda'])
\end{aligned} \tag{IV.138}$$

Corollary IV.C.1 (Hamiltonian flow)**.** *Given a function* $F(A, E)$ *over the phase space. Its Poisson bracket with the Gauss constraint* $G(\Lambda)$ *vanishes, iff* α^Λ_s*, the* Hamiltonian flow *of the Gauss constraint, is the identity map for all* $s \in \mathbb{R}$ *and* $\Lambda \in \mathfrak{su}(2)$*, i.e.:*

$$\alpha^\Lambda_s F(A, E) := \exp(s\{G(\Lambda),\ .\ \})F = \sum_{n=0}^{\infty}\frac{s^n}{n!}\{G(\Lambda), F\}_{(n)} \overset{!}{=} F(A, E) \tag{IV.139}$$

Note that the Hamiltonian flow defines an algebra isomorphism, where $\alpha^\Lambda_s(f+g) = \alpha^\Lambda_s f + \alpha^\Lambda_s g$ and $\alpha^\Lambda_s(fg) = (\alpha^\Lambda_s f)(\alpha^\Lambda_s g)$, where the first rests on linearity and the second on the Cauchy product rule and Leibniz rule: ($f^{(k)} := \partial^k_x f$)

$$(\sum_k \frac{1}{k!}f^{(k)})(\sum_l \frac{1}{l!}g^{(l)}) = \sum_n\sum_{k=0}^{n}\frac{f^{(k)}g^{(n-k)}}{k!(n-k)!} = \sum_n\sum_{k=0}^{n}\left(\begin{array}{c} n \\ k \end{array}\right)f^{(k)}g^{(n-k)} = \sum_n \frac{1}{n!}(fg)^{(n)} \tag{IV.140}$$

Also due to the Jacobi identity $\{G(\Lambda), \{f, g\}\} = \{\{G(\Lambda), f\}, g\} + \{f, \{G(\Lambda), g\}\}$ we get: $\alpha^\Lambda_s\{f, g\} = \{\alpha^\Lambda_s f, \alpha^\Lambda_s g\}$.
So we can compute its action on more involved functions, as soon as we know it on the basic variables:

Lemma IV.C.4. *Let* ($\mathbb{1}_2 := \mathrm{id}_{\mathrm{SU}(2)}$)

$$g^\Lambda_s := \exp(s\Lambda) = \cos(||\Lambda||\frac{s}{2})\mathbb{1}_2 + \frac{2\Lambda}{||\Lambda||}\sin(||\Lambda||\frac{s}{2}) \in \mathrm{SU}(2) \tag{IV.141}$$

where $||\Lambda|| = \sqrt{\delta_{IJ}\Lambda^I\Lambda^J}$ *then with* $s' = \frac{2}{\beta\kappa}s$

$$\alpha^\Lambda_{s'}A_a = -(\partial_a g^\Lambda_s)(g^\Lambda_s)^{-1} + g^\Lambda_s A_a(g^\Lambda_s)^{-1} \tag{IV.142}$$

$$\alpha^\Lambda_{s'}E^a = g^\Lambda_s E^a(g^\Lambda_s)^{-1} \tag{IV.143}$$

$$\alpha^\Lambda_{s'}F_{ab} = g^\Lambda_s F_{ab}(g^\Lambda_s)^{-1} \tag{IV.144}$$

Proof. For (IV.141) note that $\tau_I\tau_J = -\delta_{IJ}/4 + \epsilon_{IJK}\tau_K/2$ and hence $\Lambda\Lambda = -\Lambda^I\delta_{IJ}\Lambda^J/4 = -||\Lambda||^2/4$. Now

$$\sum_n \frac{s^n}{n!}\Lambda^n = \sum_n \frac{(s||\Lambda||)^{2n}}{(2n)!}(-\frac{1}{4})^{2n}\mathbb{1}_2 + \sum_n \frac{(s||\Lambda||)^{2n+1}}{(2n+1)!}(-\frac{1}{4})^{2n}\frac{\Lambda}{||\Lambda||} = \cos(||\Lambda||\frac{s}{2})\mathbb{1}_2 + \frac{2\Lambda}{||\Lambda||}\sin(||\Lambda||\frac{s}{2}) \tag{IV.145}$$

It is a straightforward calculation using (IV.134-IV.135)

$$\alpha^\Lambda_{s'}E^a = \sum_n \frac{s^n}{n!}[\Lambda, E^a]_{(n)} = \sum_n\sum_{k=0}^{n}\frac{s^n}{n!}(-)^{n-k}\begin{pmatrix} n \\ k \end{pmatrix}\Lambda^k E^a \Lambda^{n-k} = \sum_n\sum_k \frac{s^k}{k!}\Lambda^k E^a\frac{(-)^{n-k}}{(n-k)!}\Lambda^{n-k} = $$
$$= g^\Lambda_s E^a (g^\Lambda_s)^{-1} \tag{IV.146}$$
$$\alpha^\Lambda_{s'}A_a = \sum_n \frac{s'^n}{n!}(\frac{\beta\kappa}{2})^{n-1}[\Lambda,\{G(\Lambda),A_a\}]_{(n-1)} =$$
$$= -\sum_n \frac{s^n}{n!}\sum_k \begin{pmatrix} n-1 \\ k \end{pmatrix}\Lambda^k(\partial_a\Lambda)(-)^{n-1-k}\Lambda^{n-1-k} + g^\Lambda_s A_a(g^\Lambda_s)^{-1} \tag{IV.147}$$

To calculate further note that

$$\sum_{l=0}^{k}\begin{pmatrix} k \\ l \end{pmatrix}(-)^l = (1-1)^k = 0, \qquad \sum_{l=0}^{k}\begin{pmatrix} n \\ l \end{pmatrix}(-)^l = (-)^k\begin{pmatrix} n-1 \\ k \end{pmatrix} \tag{IV.148}$$

Then we find:

$$-(\partial_a\sum_k \frac{s^k}{k!}\Lambda^k)(\sum_n \frac{(-s)^n}{n!}\Lambda^n) = -\sum_n\sum_{l=0}^{n}\frac{s^l}{l!}\frac{(-s)^{n-l}}{(n-l)!}(\partial_a\Lambda^l)\Lambda n - l =$$
$$= -\sum_n \frac{s^n}{n!}\sum_{l=0}^{n}\begin{pmatrix} n \\ l \end{pmatrix}(-)^{n-l}\sum_{k=0}^{l-1}\Lambda^k(\partial_a\Lambda)\Lambda^{n-l+l-1-k} =$$
$$= -\sum_n \frac{s^n}{n!}\sum_{k=0}^{n-1}\Lambda^k(\partial_a\Lambda)\Lambda^{n-1-k}(-)^{n-1-k}\sum_{l=k+1}^{n}(-)^{k+1-l}\begin{pmatrix} n \\ l \end{pmatrix} \tag{IV.149}$$

which equals (IV.147) by $\sum_{l=k+1}^{n}(-)^{k+1-l}\begin{pmatrix} n \\ l \end{pmatrix} = \sum_{m=0}^{k}\begin{pmatrix} n \\ m \end{pmatrix}(-)^{m+1-k-1} = (-)^{k-k}\begin{pmatrix} n-1 \\ k \end{pmatrix}$. Lastly

$$\frac{2}{\beta\kappa}\{G(\Lambda),F_{ab}(x)\} = \int_\sigma d^3z(-\partial_c\Lambda^J + [\Lambda, A_c]^J)(2\partial_{[a}\delta^c_{b]}\delta^{(3)}(x,z)\tau_J + 2A^I_{[a}\delta^c_{b]}\tau_L\epsilon^{IJL}\delta^{(3)}(x,z)) =$$
$$= -2\partial_{[a}\partial_{b]}\Lambda - +\partial_{[a}[\Lambda, A_{b]}] + 2[\partial_{[b}\Lambda, A_{a]}] + 2[A_{[a},[\Lambda, A_{b]}]] =$$
$$= [\Lambda,(2\partial_{[a}A^K_{b]} + A^I_{[a}A^J_{b]}\epsilon^{IJK})\tau_K] = [\Lambda, F_{ab}] \tag{IV.150}$$

where we used that $\partial_x\delta(x-z) = -\partial_z\delta(x-z)$. From here on the computation proceeds analogously to (IV.146). □

This allows to establish for example gauge invariance of the Volume element: Using $\tau_J\tau_K = -\delta_{JK}\mathbb{1}_2/4 + \epsilon_{JKL}\tau_L/2$ we get the unique *Killing form* $k_{IJ} = k(\tau_I,\tau_J) := -2tr(\tau_I\tau_J) = \delta_{IJ}$ and that $tr(\tau_J\tau_K\tau_L) = -\epsilon_{JKL}/4$ and with this one sees that a finite gauge transformation leaves $\det(E)$ invariant:

$$\det(E) = \frac{1}{3!}\epsilon_{abc}\epsilon^{IJK}E^a_I E^b_J E^c_K \sim tr(E^aE^bE^c)\epsilon_{abc} \mapsto$$
$$\mapsto tr((gE^ag^{-1})(gE^bg^{-1})(gE^cg^{-1}))\epsilon_{abc} = tr(E^aE^bE^c)\epsilon_{abc} \tag{IV.151}$$

By $F^I_{ab}E^a_I = -2tr(F_{ab}E^a)$ combined with cyclicity of the trace, we see that the diffeomorphism constraint is already invariant under gauge transformations and a similar calculation establishes the same for the scalar constraint, i.e. it would not map out of the gauge invariant sector of the theory and no new constraints arise. However, this becomes even more apparent if we rewrite everything in a regularised version using holonomies:

Definition IV.C.5 (Holonomy)**.** *Let* $e: [0,1] \to \sigma,\ t \mapsto e(t)$ *be a piecewise analytic curve in* σ*. Let* A *be a globally defined* $\mathrm{SU}(2)$ *connection. The* holonomy $h(e) := h_t(e)\mid_{t=1}$ *of* A *along* e *is the unique solution of the ordinary differential equation (called* parallel transport equation*)*

$$\frac{d}{dt} h_t(e) = h_t(e) A_e(t) \tag{IV.152}$$

where

$$h_{t=0}(e) = \mathbb{1}_2, \qquad A_e(t) := \dot{e}^a(t) A_a^I(e(t))\tau_I \tag{IV.153}$$

Theorem IV.C.3.

1. *The explicit solution of (IV.152) is the* path ordered exponential

$$h_t(e) = \mathcal{P}\exp\left(\int_0^t ds\ A_e(s)\right) = \mathbb{1}_2 + \sum_{n=1}^{\infty} \int_0^t ds_1 \int_0^{s_1} ds_2 \ldots \int_0^{s_{n-1}} ds_n\ A_e(s_n)\ldots A_e(s_1) \tag{IV.154}$$

such that the later parameter values are always ordered to the right.

2. *The holonomy* $h(e)$ *is independent of a reparametrisation of the curve* $e \mapsto e \circ f,\ f : [a,b] \to [0,1]$ *with* $\dot{f}(t) > 0$ *for all* $t \in [a,b],\ f(a) = 0,\ f(b) = 1$*.*

3. *Under a gauge transformation of the connection (see (IV.142))*

$$A_a \mapsto A_a^g := -(dg)g^{-1} + gAg^{-1} \tag{IV.155}$$

where $g : \sigma \to \mathrm{SU}(2)$*, it holds (*$b(e) = e(0)$ *the beginning point and* $f(e) = e(1)$ *the final point of the path)*

$$h(e) \mapsto h^g(e) = g(b(e))h(e)g(f(e))^{-1} \tag{IV.156}$$

4. *Indeed, the holonomy is* $\mathrm{SU}(2)$ *valued, that is*

$$h(e)^\dagger = h(e)^{-1}, \qquad \det(h(e)) = 1 \tag{IV.157}$$

5. *Given two curves* e_1, e_2 *such that* $e_1 \cap e_2 = f(e_1) = b(e_2)$*. For the connected path*

$$(e_1 \circ e_2)(t) := \begin{cases} e_1(2t) & 0 \leq t \leq 1/2 \\ e_2(2t-1) & 1/2 \leq t \leq 1 \end{cases} \tag{IV.158}$$

and for $e^{-1}(t) := e(1-t)$*, the inversion of a curve* e*, we have respectively*

$$h(e_1 \circ e_2) = h(e_1)h(e_2), \qquad h(e^{-1}) = h(e)^{-1} \tag{IV.159}$$

Proof. For 1. we use the *Picard-Lindelöf theorem* [240] which guarantees the uniqueness of a solution of (IV.152). This leaves for us to check (IV.154)

$$\begin{aligned} \frac{d}{dt} h_t(e) &= 0 + \sum_{n=1} \left[\int_0^{s_1} ds_2 \ldots \int_0^{s_{n-1}} ds_n\ A_e(s_n)\ldots A_e(s_2)A_e(s_1)\right]_{s_1=t} = \\ &= \sum_{n=1}^{\infty} \int_0^t ds_1 \ldots \int_0^{s_{n-2}} ds_{n-1}\ A_e(s_{n-1})\ldots A_e(s_1)A_e(t) = h_t(e)A_e(t) \end{aligned} \tag{IV.160}$$

and this is indeed the path ordered exponential since it is the integration over an n-simplex [241]:

$$\mathcal{P}\left(\sum_{n=0}^{\infty} \frac{1}{n!} \int_0^t dt_1..dt_n\ A_e(t_a)..A_e(t_n)\right) = \sum_{n=0}^{\infty} \int_0^t ds_1 \ldots \int_0^{s_{n-1}} ds_n A_e(s_n)\ldots A_e(s_1) \tag{IV.161}$$

Point 2. is a simple consequence of coordinate change $s = f(t)$:

$$\int_0^1 ds \dot{e}^a(s) A_a(e(s)) \frac{\partial f}{\partial t} \dot{e}^a(f(t)) A_a(e(f(t)) = \int_a^b dt (e\circ f)'(t) A_a(e \circ f)(t)) \tag{IV.162}$$

For 3. we again use the uniqueness of solutions of

$$\frac{d}{dt}h_t^g(e) = h_t^g(e)\dot{e}^a(t)(-(dg)g^{-1} + gAg^{-1})_a(e(t)) \tag{IV.163}$$

for which we try $h_t^g(e) = g(b(e))h_t(e)g(e(t))^{-1}$ and use that $h_t(e)$ fulfils (IV.152):

$$\begin{aligned}\frac{d}{dt}h_t^g(e) &= g(b(e))(\frac{d}{dt}h_t(e))g(e(t))^{-1} + g(b(e))h_t(e)\frac{d}{dt}g(e(t))^{-1} = \\ &= g(b(e))h_t(e)g(e(t))^{-1}g(e(t))A_e(t)g(e(t))^{-1} + g(b(e))h_t(e)g(e(t))^{-1}g(e(t))\dot{e}^a(t)\frac{\partial g^{-1}}{\partial x^a}(e(t)) = \\ &= h_t^g(e)\dot{e}^a(t)(gAg^{-1})(e(t)) - h_t^g(e)\dot{e}^a(t)(\frac{\partial g}{\partial x^a}g^{-1})(e(t))\end{aligned} \tag{IV.164}$$

Since also the initial conditions remain the same $h_0^g(e) = g(b(e))\mathbb{1}_2 g(b(e))^{-1} = \mathbb{1}_2$ one obtains the claim.
We will first show 5. and consider

$$\begin{aligned}h(e_1\circ e_2) = \sum_{n=0}^{\infty}\int_0^{\frac{1}{2}} ds_1...ds_n\ A_e(s_n)...A_e(s_1) + \int_{\frac{1}{2}}^1 ds_1(\sum_{n=0}\int_0^{\frac{1}{2}} ds_2..ds_n A_e(s_n)..A_e(s_2))A_e(s_1) + \\ + \int_{\frac{1}{2}}^1 ds_1\int_{\frac{1}{2}}^{s_1} ds_2(\sum_{n=0}\int_0^{\frac{1}{2}} ds_3..A_e(s_3))A_e(s_2)A_e(s_1) + ... = \\ = h(e_1)\left(\mathbb{1}_2 + \int_{\frac{1}{2}}^1 ds_1 A_e(s_1) + \int_{\frac{1}{2}}^1 ds_1\int_{\frac{1}{2}}^{s_1} ds_2\ A_e(s_2)A_e(s_1) + ...\right) = h(e_1)h(e_2)\end{aligned} \tag{IV.165}$$

To show the second point of 5., consider

$$A_{e^{-1}}(t) = (e^{-1})^{\cdot}(t)A_a(e^{-1}(t) = -\dot{e}(1-t)A_a(e(1-t)) = -A_e(1-t) \tag{IV.166}$$

which implies

$$\int_0^1 ds_1...\int_0^{s_{n-1}} ds_n A_{e^{-1}}(s_n)...A_{e^{-1}}(s_1) = (-)^n\int_0^1 dt_1...\int_{t_{n-1}}^1 dt_n A_e(t_n)...A_e(t_1) \tag{IV.167}$$

To shorten the notation we introduce $\mathcal{A}_a^b(s) := \int_a^b dt A_e(t)$. Now

$$h(e)h(e^{-1}) = 1 + \mathcal{A}_0^1(s_1) - \mathcal{A}_0^1(t_1) + \sum_{n=2}^{\infty}(-)^n\sum_{k=0}^{n}(-)^k\mathcal{A}_0^{s_{k_1}}(s_k)...\mathcal{A}_0^1(s_1)\mathcal{A}_{t_{n-k-1}}^1(t_{n-k})... \tag{IV.168}$$

For $n \geq 2$:

$$\begin{aligned}&\mathcal{A}_t^1 n.1(t_n)...\mathcal{A}_0^1(t_1) - \mathcal{A}_0^1(s)\mathcal{A}_{t_{n-2}}^1(t_{n-1})...\mathcal{A}_0^1(t_1) + \sum_{k=2}^{n}... = \\ &= \mathcal{A}_{t_{n-1}}^1(t_n)...\mathcal{A}_0^1(t_1) - (\mathcal{A}_{t_{n-1}}^1(s)\mathcal{A}_{t_{n-2}}^1(t_{n-1}) + \mathcal{A}_0^{t_{n-1}}(s)\mathcal{A}_{t_{n-2}}^1(t_{n-1}))...\mathcal{A}_0^1(t_1) + \sum_{k=2}^{n}... = \\ &= -\mathcal{A}_0^{s_1}(s_2)\mathcal{A}_{t_{n-2}}^1(s_1)\mathcal{A}_{t_{n-3}}^1(t_{n-2})...\mathcal{A}_0^1(t_1) + \sum_{k=2}^{n}...\end{aligned} \tag{IV.169}$$

We iterate, from $k \to k+1$:

$$\begin{aligned}&(-)^{k-1}\mathcal{A}_0^{s_{k-1}}(s_k)...\mathcal{A}_{t_{n-k}}^1(s_1)\mathcal{A}_{t_{n-k-1}}^1(t_{n-k})...\mathcal{A}_0^1(t_1) + (-)^k\mathcal{A}_0^{s_{k-1}}(s_k)...\mathcal{A}_0^1(s_1)\mathcal{A}_{t_{n-k-1}}^1(t_{n-k})... = \\ &= (-)^k\mathcal{A}_0^{s_{k-1}}...(-\mathcal{A}_{t_{n-k}}^1(s_1)\mathcal{A}_{t_{n-k-1}}^1(t_{n-k}) + \mathcal{A}_0^1(s_1)\mathcal{A}_{t_{n-k-1}}^1(t_{n-k}))... = \\ &= (-)^k\mathcal{A}_0^{s_k}(s_{k+1})...\mathcal{A}_0^{s_1}(s_2)\mathcal{A}_{t_{n-(k+1)}}^1(s_1)\mathcal{A}_{t-(k+1)-1}^1(t_{n-(k+1)})...\mathcal{A}_0^1(t_1)\end{aligned} \tag{IV.170}$$

Thus, all powers of $n \neq$ vanish separately and it follows $h(e^{-1}) = h(e)^{-1}$.
Lastly, 4. follows from the initial condition $h_{t=0}(e) = \mathbb{1}_2$ and (remember (IV.45))

$$\frac{d}{dt}\det(h_t(e)) = \det(h_t(e))tr(h_t(e)^{-1}\frac{d}{dt}h_t(e)) = \det(h_t(e))tr(A_e(t)) = 0 \Rightarrow 1 = \det(h_0(e)) = \det(h_t(e)) \tag{IV.171}$$

and remembering that $\tau_J^\dagger = -\tau_J$ for $J = 1...3$

$$h(e)^\dagger = \sum_{n=0}^{\infty} \int ... \int ds_n \; (A_e(s_n)...A_e(s_1))^\dagger = \sum_{n=0}^{\infty} \int ... \int ds_n \; A_e^{J_1}(s_1)\tau_{J_1}^\dagger ... A_c^{J_n}(s_n)\tau_n^\dagger$$
$$= \sum_{n=0}^{\infty} (-)^n \int ... \int ds_n \; A_e(s_1)..A_e(s_n) \tag{IV.172}$$

which is exactly $h(e^{-1})$ as one can see by a similar iteration as for $h(e^{-1})$ and the simplex argument for (IV.161). □

Theorem IV.C.4 (Non-Abelian Stokes theorem)**.** *(cf. [50, 242] for example) The complete information about the connection is contained the set of all holonomies: Given a curve e we define $e_\epsilon(t) := e(t\epsilon)$ for $0 < \epsilon < 1$. Then:*

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon}(h(e_\epsilon) - \mathbb{1}_2) = A_e(t = 0) \tag{IV.173}$$

Also, curvature can be expressed in terms of holonomies: Consider a closed path (loop) assuming the form of a plaquette at $x = e^u(0) \in \sigma$

$$\Box^\epsilon_{x,uv}(t) := e^u_\epsilon \circ e^{v\epsilon}_\epsilon \circ (e^{u\epsilon}_\epsilon)^{-1} \circ (e^v_\epsilon)^{-1} \tag{IV.174}$$

where $u = \dot{e}^u(0) = \dot{e}^{u\epsilon}(0)$ and $v = \dot{e}^v(0) = \dot{e}^{v\epsilon}(0)$[12]. For the concatenation to be well defined we have to demand that the different paths have connected start/end points, i.e. $e^u_\epsilon(1) = e^{v\epsilon}_\epsilon(0)$, and so forth until $e^v_\epsilon(0) = \epsilon^u_\epsilon(0)$. If $[u, v] = 0$ one gets

$$\lim_{\epsilon \to 0} \frac{1}{2\epsilon^2}(h(\Box^\epsilon_{x,uv}) - h(\Box^\epsilon_{x,uv})^{-1}) = \lim_{\epsilon \to 0} \frac{1}{\epsilon^2}(h(\Box^\epsilon_{x,uv}) - \mathbb{1}_2) = u^a v^b F_{ab}(x) \tag{IV.175}$$

Proof. Using the theorem of monotone convergence [243]:

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon}(-\mathbb{1}_2 + h(e_\epsilon)) = \lim_{\epsilon \to 0} \frac{1}{\epsilon}(-\mathbb{1}_2 + \mathbb{1}_2 + \sum_{n=1} \epsilon^n \int_0^1 ds_1 ... \dot{e}^a(s_1\epsilon) A_a^{J_1}(e(s_1\epsilon))\tau_{J_1}...) =$$
$$= \lim_{\epsilon \to 0} \int_0^1 ds \dot{e}^a(s\epsilon) A_a^J(s\epsilon)\tau_J + \mathcal{O}(\epsilon) = \int_0^1 ds \dot{e}^a(0) A_a^J(0)\tau_J = A_e(t = 0) \tag{IV.176}$$

and the second claim we establish in the following way: by cutting the path ordered exponential of each of the four holonomies after the first two terms in the series. Then for the terms linearly depending on A_e we perform a power series expansion in s which stops at linear order, and respectively for the quadratic terms the expansion is in terms of $(s_1, s_2)/(s, t)$ stopping at zeroth order:

$$\begin{aligned}
&\lim_{\epsilon \to 0} \frac{1}{\epsilon^2}(h(e^u)h(e^{v\epsilon}_\epsilon)h^{-1}(e^{u\epsilon}_\epsilon)h^{-1}(e^v) - \mathbb{1}_2) = \\
&= \lim_{\epsilon \to 0} \frac{1}{\epsilon^2}\Big(\int_0^\epsilon ds \dot{e}^u(s)^a A_a(e(s)) + \int_0^\epsilon ds [\dot{e}^{v\epsilon}_\epsilon(0)^a A_a(e^{v\epsilon}_\epsilon(0)) + d\frac{d}{dt}(\dot{e}^{v\epsilon}_\epsilon(t)^a A_a(\tilde{c}^{v\epsilon}_\epsilon(t)) \mid_{t=0}] + \\
&\quad + \epsilon(\dot{e}^{u\epsilon}_\epsilon)^{-1}(0)^a A_a((e^{u\epsilon}_\epsilon)^{-1}(0)) + \frac{\epsilon^2}{2}[(\dot{e}^{u\epsilon}_\epsilon)^{-1}(t)^b(\partial_b(\dot{e}^{u\epsilon}_\epsilon)^{-1}(t)^a)A_a((e^{u\epsilon}_\epsilon)^{-1}(t))]_{t=0} + \\
&\quad + \epsilon(-v(x + \epsilon v)^a)A_a(x + \epsilon v) + \frac{\epsilon^2}{2}[v(x)^b(v(x)^a)A_a(x) + v(x)^a v(x)^b \partial_b A_a(x)] + \\
&\quad + \int_0^\epsilon ds_1 \int_0^{s_1} ds_2 \; \dot{e}^u(s_1)^a A_a(e^u(s_1))\dot{e}^u(s_2)^b A_b(e^u(s_2)) + \\
&\quad + \int_0^\epsilon ds_1 \int_0^{s_1} ds_2 \; [\dot{e}^{v\epsilon}_\epsilon(0)^a A_a(e^{v\epsilon}_\epsilon(0))\dot{e}^{v\epsilon}_\epsilon(0)^b A_b(e^{v\epsilon}_\epsilon(0))] + \\
&\quad + \frac{\epsilon^2}{2}(-u(x + \epsilon v + \epsilon u)^a)(-u(x + \epsilon v + \epsilon u)b)A_y(x)A_b(x) + \frac{\epsilon^2}{2}v^a v^b A_a(x)A_b(x) + \\
&\quad + \int_0^\epsilon ds \int_0^\epsilon dt \; \dot{e}^u(s)^a A_a(e^a(s))\dot{e}^{v\epsilon}_\epsilon(t)^b A_b(c^{v\epsilon}_\epsilon(t)) + \epsilon^2 u(x)^a(-u(x + \epsilon u + \epsilon v)^b A_a(x)A_b(x) + \\
&\quad + \epsilon^2(-u^a v^b - v^a u^b - v^a v^b + u^a v^b)A_a A_b\Big) = \\
&= u^b(\partial_b v^a)A_a(x) - v^b(\partial_b u^a)A_a(x) - v^b u^a \partial_b A_a(x) + v^a u^b \partial_b A_a(x) + (-v^a u^b + u^a v^b)A_a(x)A_b(x) = \\
&= [u, v]^a A_a(x) + u^a v^b 2\partial_{[a}A_{b]} + u^a v^b [A_a(x), A_b(x)] = u^a v^b F_{ab}(x)
\end{aligned} \tag{IV.177}$$

[12] The extra ϵ dependence in the paths $e^{u\epsilon}, e^{\epsilon v}$ is due to the fact that they are supposed to form a loop.

where we used $[u,v]=0$ in the last step. Finally use antisymmetry, i.e. $F_{ab}u^a v^b - F_{ab}v^a u^b = 2F_{ab}u^a v^b$. □

Definition IV.C.6 (Faces, electric fluxes)**.** *A face S is a finite union of connected, entire analytic embedded 2-dimensional submanifolds S_I of σ, whose closures intersect at most in their boundaries, which are themselves piecewise analytic paths, and are such that S is orientable ($\exists\ U \supset S$ such that $U - S = U_1 \cup U_2$ where U_1, U_2 are disjoint non-empty open sets). Moreover, we demand the closure of S to be contained in a compact set.*
Let f be a Lie-algebra valued, scalar function of compact support. The corresponding electric flux *of the vector density E^a_J through a face S is defined by*

$$E_f(S) := \int_S f^J * E_J = \int_s dx^a \wedge dx^b\ \epsilon_{abc} E^c_J f^J \tag{IV.178}$$

Following a strategy from [154], we restrict the set of all possible paths e and faces S to a subset, where for each path e therein one can assign a face S_e carrying the same orientation as e such that (1) the faces S_e are mutually non-intersecting, (2) only e intersects S_e and (3) this intersection happens only in one point and is transversal. While one could also consider the general set of *all* paths and faces, for the purpose of this chapter the mentioned subset will be sufficient and, in an abuse of notation, we will still call it the *holonomy-flux algebra*.

Lemma IV.C.5 (Holonomy-flux Poisson bracket)**.** *Consider a holonomy $h(e)$ and an electric flux $E_f(S)$ such that S is intersected transversal by $e = e_1 \circ e_2$ with $e_i \in U_i$. The Poisson bracket between both is:*

$$\{E_f(S), h(e)\} = \frac{\beta\kappa}{2}\sigma(S,e)h(e_1)\tau_J h(e_2) f^J(S\cap e) \tag{IV.179}$$

where $\sigma(S,e) = +1$ if the tangent of e points upwards with respect to the conormal of the surface at the intersection point and -1 otherwise.[13]

Proof. We write $e = e_1^\epsilon \circ e_\epsilon \circ e_2^\epsilon$ such that e_ϵ is the segment including the intersection point $S\cap e$. Consider embeddings (with $e(\frac{1}{2}) = S(0,0) = e\cap S$)

$$S : (-1,1)^2 \to \sigma\ :\ (u,v) \mapsto S(u,v), \qquad\qquad e_\epsilon : (\frac{1}{2}-\epsilon, \frac{1}{2}+\epsilon) \to \sigma\ :\ t \mapsto e(t) \tag{IV.180}$$

Then compute by expanding $h(e_\epsilon)$ in terms of ϵ:

$$\begin{aligned}
\{E_f(S), h(e)\} &= \lim_{\epsilon\to 0} h(e_1^\epsilon)\{E_f(S), \mathbb{1}_2 + \int_0^1 ds A_{e_\epsilon}(s) + \mathcal{O}(\epsilon^2)\}h(e_2^\epsilon) = \qquad\qquad (\text{IV.181})\\
&= \lim_{\epsilon\to 0} h(e_1^\epsilon)\int_{(-1,1)^2} dudv\ \epsilon_{abc}\frac{\partial S^b}{\partial u}\frac{\partial S^c}{\partial v} f^J(S(u,v)) \int_{\frac{1}{2}-\epsilon}^{\frac{1}{2}+\epsilon} dt\ \dot{e}^d(t)\{E^a_J(S(u,v)), A_d(e(t))\} h(e_2^\epsilon) = \\
&= \frac{\beta\kappa}{2}\lim_{\epsilon\to 0} h(e_1^\epsilon)\int dtdudv\ \dot{e}^a(t)\frac{\partial S^b}{\partial u}\frac{\partial S^c}{\partial v}\epsilon_{abc}\tau_k f^k(S(u,v))\delta^3(e(t)-S(u,v))h(e_2^\epsilon) = \\
&= \frac{\beta\kappa}{2}\lim_{\epsilon\to 0} h(e_1^\epsilon)\int d^3x\delta^3(x)\frac{\det(\dot{e}(t), -S_{,u}, -S_{,v})}{|\ \dot{e}, S_{,u}, S_{,v}\ |}\tau_J h(e_2^\epsilon) f^J(S\cap e) = \frac{\beta\kappa}{2}\sigma(s,e)h(e_1^0)\tau_J h(e_2^0) f^J(S\cap e)
\end{aligned}$$

where we performed the coordinate change $t,u,v \mapsto x(t,u,v) = e(t) - S(u,v)$ for the fourth line, which gave us as Jacobian the absolute value of the inverse determinant. □

Corollary IV.C.2 (Regularised scalar constraint)**.** *In terms of holonomies we can circumvent to choose any coordinate chart and due to their nice transformation under* SU(2) *we find the manifestly* SU(2) *invariant formulation for the scalar constraint as the limit $C[N] = \lim_{\epsilon\to 0} C^\epsilon[N]$ (note $\int d^3x = \lim_{\epsilon\to 0}\sum_{\square\in T(\epsilon)}\epsilon^3$) with*

$$\begin{aligned}
C^\epsilon[N] &:= C^\epsilon_E[N] + \frac{4^3(1+\beta^2)}{\kappa^4\beta^7}\sum_{v\in T(\epsilon)} N(v)\sum_{ijk}\frac{\epsilon(i,j,k)}{T_v}\times \\
&\times tr\left(h(e_i)\{h(e_i)^\dagger, \{V, C^\epsilon_E[1]\}\}h(e_j)\{h^\dagger(e_j), \{V, C^\epsilon_E[1]\}\}h(e_k)\{h^\dagger(e_k), V_\epsilon(v)\}\right) \qquad (\text{IV.182})\\
C^\epsilon_E[N] &:= \frac{-4}{\kappa^2\beta}\sum_{v\in T(\epsilon)} N(v)\sum_{ijk}\frac{\epsilon(i,j,k)}{T_v} tr\left((h(\square^\epsilon_{v,ij}) - h^\dagger(\square^\epsilon_{v,ij}))h(e_k)\{h^\dagger(e_k), V_\epsilon[\sigma]\}\right) \qquad (\text{IV.183})
\end{aligned}$$

[13] Due to those smearings the distributional character of the Poisson bracket is lost and, moreover, one has a background independent formulation for the algebra, as the right-hand side does not depend on the metric.

where $T(\epsilon)$ is some cubulation of σ. Its dual is a lattice with six-valent vertices v such that for each vertex one can associate one cell. The volume of each cell, $V_\epsilon(v)$, vanishes for $\epsilon \to 0$. Also we defined $V_\epsilon[\sigma] := \sum_v V_\epsilon(v)$. $T_v = 2^3$ is number of all contributing triples of edges e_i which meet at v. By this, we mean those triples for which $\epsilon(i,j,k) := sgn(\det(\dot{e}_i, \dot{e}_j, \dot{e}_k))$ does not vanish. Lastly, we have labelled all adjacent edges of v as outgoing.

Proof. We only sketch the main steps, for all details consult [50, 74, 75]. Consider C_E. Note, that we can express $\delta_{IJ}/2 = -2\, tr(\tau_I\tau_J)$ and $\epsilon_{IJK} = -4\, tr(\tau_I\tau_J\tau_K)$ to obtain

$$C_E(x) = \frac{4}{\kappa^2\beta} tr(F_{ab}(x)\epsilon^{abc}\{V, A_c(x)\}) \tag{IV.184}$$

First, we approximate the Integral by a sum over all cells of the mentioned cubulation, labelled by v. Then for all x in cell v

$$\epsilon^{abc}F_{ab}(x) \approx \epsilon^{abc}F_{ab}(v) + \mathcal{O}(\epsilon) = \epsilon^{abc}\frac{2^3 F_{ab}(v)}{2^3} + \mathcal{O}(\epsilon) = \frac{1}{2^3}\sum_{ijk}(\dot{e}_k)^c \epsilon(i,j,k) F_{ab}(\dot{e}_i)^a(\dot{e}_j)^b + \mathcal{O}(\epsilon) \tag{IV.185}$$

where we chose the tangent vectors to have absolute value 1. Now, we plug in (IV.175) and ($\dot{e} = \vec{e}_a\epsilon$)

$$\begin{aligned} h(e)\{h(e)^\dagger, V\} &= (\mathbb{1}_2 + \epsilon\int_0^1 dt\dot{e}^c(t)A_c(e(t)) + \mathcal{O}(\epsilon^2))\{\mathbb{1}_2 - \epsilon\int_0^1 dt\dot{e}_c(t)A_c(e(t)) + \mathcal{O}(\epsilon^2), V^\epsilon[\sigma]\} = \\ &= -\epsilon\int_0^1 dt\,\{A_a(t\epsilon\vec{e}_a), V^\epsilon[\sigma]\} = \epsilon\int_0^1 dt\,\delta_{\vec{e}_a(t)\in S_{e_a}}\frac{\beta\kappa}{2}\frac{\delta V^\epsilon[\sigma]}{\delta E_I(S_e)}\tau_I = -\epsilon\{A_a(e(0)), V\} + \mathcal{O}(\epsilon^2) \end{aligned} \tag{IV.186}$$

to obtain the claim. Note that we used: $\delta V^\epsilon[\sigma]/\delta E_I(S_e) \approx \delta V/\delta E_I(e(0)) + \mathcal{O}(\epsilon)$.
For $C \approx C^\epsilon + \mathcal{O}(\epsilon)$ we proceed similar. □

IV.D Example: Cosmological Models

To illustrate the rather involved nature of the previous sections, we will now have a look at a concrete example. This will put the formalism developed so far into action. We present how calculations therein are explicitly performed and make contact with physical observations. The chosen example for this section is one of the few completely analytically solvable models, which also bears significant physical importance: *isotropic cosmology* described by the Friedmann-Lemaître-Robertson-Walker (FRLW) metric [22–31].
By this we mean spacetimes, whose spatial hypersurfaces (according to the cosmological principle) have a high degree of symmetries, i.e. the metric on them is invariant under translations and rotations. In other words, there is no preferred point or direction in the spatial slice. The observable universe appears to be subject to those spatial symmetries at large scales and hence these models have led to several predictions, which could be verified with high precision. Most prominent among them is the Big Bang singularity and the cosmic microwave background [20]. There are excellent textbooks covering this subject, e.g, [32, 244, 245], so we will only give a brief overview.

IV.D.1 Robertson-Walker metric & Killing fields

We start by giving a precise mathematical meaning to the condition "being invariant under spatial translations and rotations", which obviously will be connected to the notion of diffeomorphisms (see Definition IV.A.3). For the moment we consider only a subset, namely those which for a given spatial metric q leave the latter invariant, i.e. in a given coordinate chart $x : \sigma \to \mathbb{R}^3$

$$\varphi : U \to \sigma, \qquad q = \varphi^* q, \qquad q_{ab}(x(p)) = \frac{\partial\varphi(x(p))^c}{\partial x^a}\frac{\partial\varphi(x(p))^d}{\partial x^b}q_{cd}(\varphi(x(p))) \tag{IV.187}$$

In which case we will call φ an *isometry* (of the spatial metric). If for each pair of points $p, p' \in \sigma$ there exists such an isometry with $\varphi(p) = p'$ then we call a space *homogeneous*, which corresponds to invariance under translations. Similarly, in order to incorporate invariance under rotations, we call a pair (σ, q) *isotropic*, iff at any point $p \in \sigma$ we find for all unit vectors $v_1, v_2 \in T^1(\sigma)$ with $q_{ab}v_i^a v_i^b = 1$ an isometry φ with $\varphi(p) = p$ and $\varphi(v_1) = v_2$. The latter property indicates that φ belongs to the subspace of diffeomorphisms that leaves

p invariant and is isomorphic to $SO(3)$, i.e. the group of three-dimensional special orthogonal transformations which leave p invariant.
Given φ_t, a one-parameter group of such isometries, $t \in \mathbb{R}$, with the properties that $\varphi_t \circ \varphi_s = \varphi_{t+s}$ and hence $\varphi_0 = \mathrm{id}_\sigma$. Then there is a unique way to invert (IV.22) and find a tangential vector, k, for this parameter group by looking at its infinitesimal action. Let $\epsilon \ll 1$ then we define:

$$\varphi_\epsilon(x(p))^a =: x(p)^a + \epsilon k^a(x(p)) + \mathcal{O}(\epsilon^2) \tag{IV.188}$$

As usual we omit in the following the dependence of $x := x(p)$. In first order in ϵ we can express (IV.187) as

$$q_{ab} = (\delta_a^d + \epsilon\frac{\partial k^d}{\partial x^a})(\delta_b^e + \epsilon\frac{\partial k^e}{\partial x^b})(q_{de} + \epsilon k^c\frac{\partial q_{de}}{\partial x^c}) + \mathcal{O}(\epsilon^2) \;\;\Rightarrow\;\; 0 = \frac{\partial k^c}{\partial x^a}q_{cb} + \frac{\partial k^c}{\partial x^b}q_{ac} + k^c\frac{\partial q_{ab}}{\partial x^c} \tag{IV.189}$$

By introducing $k_a := q_{ab}k^b$ and remembering the (spatial) Christoffel symbols (IV.29) this is equivalent to

$$0 = \frac{\partial k_a}{\partial x^b} + \frac{\partial k_b}{\partial x^a} + k^c(\frac{\partial q_{ab}}{\partial x^c} - \frac{\partial q_{cb}}{\partial x^a} - \frac{\partial q_{ac}}{\partial x^b}) = 2\partial_{(a}k_{b)} - 2\Gamma^c_{ab}k_c\,. \tag{IV.190}$$

Remembering metric compatibility $Dq = 0$ for a (spatial) Lie derivative (IV.27), we obtain the *Killing equation*:

$$\mathcal{L}'_k q_{ab} = 2q_{c(a}D_{b)}k^c = D_{(a}k_{b)} = 0 \tag{IV.191}$$

and every vector field k_a fulfilling it - and thus being in 1-1 correspondence with an isometry group φ_t - is called a *Killing vector*.

As we are interested in spaces with a high degree of symmetry, one would assume that we are looking for those with the maximal number of linear independent Killing vectors. Indeed, one can show that there are at most $n(n+1)/2$ many Killing fields in a manifold with $\dim\sigma = n$. Moreover, a space with this maximal number of Killing fields will be automatically isotropic and homogeneous. Hence, it is sufficient to find the full set of Killing vectors in order to determine that a spacetime is a suitable candidate for our large-scale universe. We will make this now precise by determining the six Killing vectors of the so-called *Robertson-Walker* metric and hence proving it to describe a spatially isotropic and homogeneous universe:

$$g_k := -dt^2 + a(t)^2\left(\frac{1}{1-kr^2}dr^2 + r^2d\theta^2 + r^2\sin(\theta)^2d\phi^2\right) \tag{IV.192}$$

where $k \in \{0, \pm 1\}$ and $a(t)$ is function just depending on the foliation parameter t, called the *scale factor*. Also we have used spherical coordinates: $\theta \in [0,\pi), \phi \in [0, 2\pi)$ and $r \in [0,1)$ if $k = +1$ else $r \in \mathbb{R}_+$.

However, to find its Killing vectors it is easier to transform into Cartesian coordinates, i.e. we introduce $x^i(r,\theta,\phi) \in \mathbb{R}$ with

$$x^1 = r\sin(\theta)\cos(\phi), \qquad x^2 = r\sin(\theta)\sin(\phi), \qquad x^3 = r\cos(\theta) \tag{IV.193}$$

Using that $\sin(a)^2 + \cos(a)^2 = 1$, one can easily see that under a coordinate change as in (IV.10):

$$\begin{aligned}\delta_{ij}dx^idx^j =&(dx^1)^2 + (dx^2)^2 + (dx^3)^2 = (\sin(\theta)\cos(\phi)dr + r\cos(\theta)\cos(\phi)d\theta - r\sin(\theta)\sin(\phi)d\phi)^2 + \\ &+ (\sin(\theta)\sin(\phi)dr + r\cos(\theta)\sin(\phi)d\theta + r\sin(\theta)\cos(\phi)d\phi)^2 + (\cos(\theta)dr - r\sin(\theta)d\theta)^2 \\ =&(\sin\theta^2\cos\phi^2 + \sin\theta^2\sin\phi^2 + \cos\theta^2)dr^2 + r^2(\cos\theta^2\cos\phi^2 + \cos\theta^2\sin\phi^2 + sin\theta^2)d\theta^2 + \\ &+ r^2(\sin\theta^2\sin\phi^2 + \sin\theta^2\cos\phi^2)d\phi^2 = dr^2 + r^2\sin\theta^2d\phi^2 + r^2d\theta^2\end{aligned} \tag{IV.194}$$

and ($r^2 = (x^1)^2 + (x^2)^2 + (x^3)^2$)

$$\begin{aligned}\frac{(\delta_{ij}x^idx^j)^2}{1-k\delta_{lm}x^lx^m} =& \frac{1}{1-kr^2}\big((r\sin\theta^2\cos\phi^2dr + r^2\sin\theta\cos\phi^2\cos\theta d\theta - r^2\sin\theta^2\cos\phi\sin\phi d\phi) \\ &+(r\sin\theta^2\sin\phi^2dr + r^2\sin\theta\sin\phi^2\cos\theta d\theta + r^2\sin\theta^2\sin\phi\cos\phi d\phi) + (r\cos\theta^2dr - r^2\cos\theta\sin\theta d\theta)\big)^2 \\ =& \frac{1}{1-kr^2}\left(rdr + r^2(\sin\theta\cos\theta(\cos\phi^2 + \sin\phi^2) - \sin\theta\cos\theta)d\theta\right)^2 = \frac{r^2dr^2}{1-kr^2}\end{aligned} \tag{IV.195}$$

Plugging both together we realise that the Robertson-Walker metric from (IV.192) reads explicitly

$$g_k = -dt^2 + a(t)^2\left(\delta_{ij}dx^idx^j + \frac{k}{1-kr^2}(\delta_{ij}dx^idx^j)^2\right) \tag{IV.196}$$

If we call the spatial part $q_{ab} := a^2\delta_{ab} + \frac{a^2k}{1-kr^2}x^ax^b$ we can find its inverse $q^{ab} = (\delta^{ab} - kx^ax^b)/a^2$ since

$$q^{ab}q_{bc} = \delta^a_c - kx^ax^c + \frac{k}{1-kr^2}x^ax^c - \frac{k^2}{1-kr^2}x^ax^c(x^bx^b) = \delta^a_c - kx^ax^c + kx^ax^c\frac{1-kr^2}{1-kr^2} = \delta^a_c \quad \text{(IV.197)}$$

It is instructive to compute $\Gamma(q)$, the (spatial) Christoffel symbols of the purely spatial part, i.e. q, with (IV.29):

$$\partial_a q_{bc} = \frac{a^2k}{1-kr^2}2\delta^{(j}_a x^{i)}\delta_{bi}\delta_{cj} + \frac{2a^2k}{1-kr^2}\delta_{ib}\delta_{ak}\delta_{cj}x^ix^jx^k = \quad \text{(IV.198)}$$

$$= \frac{a^2k}{1-kr^2}\left(\delta_{cj}x^j(\delta_{ab} + k\frac{\delta_{ib}\delta_{ja}x^ix^j}{1-kr^2}) + x^j\delta_{jb}(\delta_{ac} + k\frac{\delta_{ai}x^i\delta_{ck}x^k}{1-kr^2})\right) = \frac{2k}{1-kr^2}q_{a(b}\delta_{c)j}x^j$$

$$\Gamma^a_{bc}(q) = \frac{1}{2}q^{ad}(2\partial_{(b}q_{c)d} - \partial_d q_{bc}) = \frac{k}{1-kr^2}q^{ad}\left(q_{b(c}\delta_{d)j} + q_{c(b}\delta_{d)j} - q_{d(b}\delta_{c)j}\right)x^j = \frac{k}{a^2}q_{bc}x^a \quad \text{(IV.199)}$$

by which we get full computational control over the spatial metric. E.g. with these at hand we can check that the Killing vector fields corresponding to rotations in the mn-plane, called $k_{[mn]}$, and those corresponding to translations in direction m, called k_m, are given by

$$k_{[mn]} := x^i\delta_{i[m}\partial_{n]}, \qquad k_m := \sqrt{1-kr^2}\partial_m \quad \text{(IV.200)}$$

To show this we use several times $q_{ab}/a^2 = \delta_{ab} + \frac{k}{1-kr^2}x^ax^b$ in (IV.191) and realise that $k^c_{[mn]}\delta_{cj}x^j = 0$:

$$\partial_{(a}(q_{b)c}k^c_{[mn]}) - \Gamma^c_{ab}(q)q_{cd}k^d_{[mn]} = a^2\delta_{i[m}\delta^c_{n]}\delta^i_{(a}(\delta_{b)c} + \frac{k}{1-kr^2}\delta_{b)j}\delta_{ck}x^jx^k) + \quad \text{(IV.201)}$$

$$+ \frac{k}{1-kr^2}(q_{ab}\delta_{cj}x^jk^c_{[mn]} + q_{c(a}\delta_{b)j}x^jk^c_{[mn]}) - kq_{ab}x^ck^d_{[mn]}(\delta_{cd} + \frac{k}{1-kr^2}\delta_{ci}\delta_{dj}x^ix^j) =$$

$$= \frac{a^2k}{1-kr^2}(x^j\delta_{j(b}\delta_{a)[m}\delta_{n]k}x^k + x^k\delta_{k[m}\delta^c_{n]}\delta_{c(a}\delta_{b)j}x^j + \frac{k}{1-kr^2}x^i\delta_{i(b}\delta_{a)k}x^kk^c_{[mn]}\delta_{cj}x^j) = 0$$

and with $(1-kr^2)x^j(\delta_{jm} + \frac{k}{1-kr^2}\delta_{ji}x^i\delta_{mk}x^k) = x^j\delta_{jm}$ also

$$\partial_{(a}(q_{b)c}k^c_m) - \Gamma^c_{ab}(q)q_{cd}k^d_m = \frac{k\,k^c_m}{1-kr^2}(q_{ab}\delta_{cj}x^j + q_{c(a}\delta_{b)j}x^j) - k\frac{x^j\delta_{j(a}q_{b)m}}{\sqrt{1-kr^2}} - \frac{k}{a^2}\sqrt{1-kr^2}q_{ab}x^cq_{cm}$$

$$= \frac{k}{\sqrt{1-kr^2}}x^j(q_{ab}\delta_{mj} + q_{m(b}\delta_{a)j} - \delta_{j(a}q_{b)m} - \frac{q_{jm}}{a^2}q_{ab}(1-kr^2)) = 0 \quad \text{(IV.202)}$$

With this we have found the maximal set of six Killing vector fields for each three dimensional spatial hypersurface, hence the Robertson-Walker metric g_k for each $k \in \{0, \pm 1\}$ indeed describes a homogeneous and isotropic universe.[14]

Since we have computed the spatial Christoffel symbols above, it is easy to verify further physical properties of this spacetime, e.g. that it is of constant curvature k everywhere; as when computing the Ricci tensor (IV.35):

$$R_{ab} = -2\partial_{[a}\Gamma^c_{c]b}(q) + 2\Gamma^d_{b[a}(q)\Gamma^c_{c]d}(q) = \frac{k}{a^2}q_{ab}(3-1) - \frac{k^2a^{-2}}{1-kr^2}(x^c2q_{[ac]}\delta_{bj}x^j + q_{ba}r^2 - x^cq_{cb}\delta_{aj}x^j) +$$

$$+ \frac{k^2}{a^2}(q_{ab}r^2 - x^cq_{cb}x^d\delta_{da})(1 + \frac{kr^2}{1-kr^2}) = 2kq_{ab}/a^2 \quad \text{(IV.203)}$$

and consequently $R = 6k/a^2$ on the whole σ.[15]

We finish this section by another coordinate transformation, whose details are due to [248]. Namely upon defining $r =: S_k(\tilde{r}) = \frac{1}{\sqrt{\kappa}}\sin(\sqrt{\kappa}\tilde{r})$ one shows easily from (IV.192) calling $d\Omega^2 := (d\theta^2 + \sin\theta^2 d\phi^2)$ that

$$q = \frac{dr^2}{1-kr^2} + r^2d\Omega^2 = \frac{\cos(\sqrt{k}\tilde{r})^2}{1-\sin(\sqrt{k}\tilde{r})^2}d\tilde{r}^2 + S_k(\tilde{r})^2d\Omega^2 = d\tilde{r}^2 + S_k(\tilde{r})^2d\Omega^2 \quad \text{(IV.204)}$$

[14] Moreover, these three are the only possible cases for an isotropic universe. However, as we are only interested in some example we refrain from presenting this proof here and refer instead to the literature [246, 247].

[15] Take note that this is only the spatial Ricci scalar of the hypersurface. For $R^{(4)}$ as appearing in the Einstein field equation (IV.43) we have to repeat the above calculations with the four dimensional covariant derivative ∇. (see next paragraph)

Lastly, we change $r' := 2\tan(\sqrt{k}\tilde{r}/2)/\sqrt{k}$ and remember $\partial_x \tan(x) = 1/\cos(x)^2$ as well as $\sin(2x) = 2\sin(x)\cos(x)$ for

$$\frac{1}{(1+\frac{k}{4}r'^2)^2}\left(dr'^2 + r'^2 d\Omega^2\right) = \frac{1}{(1+\tan(\sqrt{k}\tilde{r}/2)^2)^2}\left(\frac{d\tilde{r}^2}{\cos(\tilde{r})^4} + \frac{4}{k}\tan(\sqrt{k}\tilde{r}/2)^2 d\Omega^2\right) =$$
$$= d\tilde{r}^2 + \frac{1}{k}(2\sin(\sqrt{k}\tilde{r}/2)\cos(\sqrt{k}\tilde{r}/2))^2 d\Omega^2 = d\tilde{r}^2 + S_k(\tilde{r})^2 d\Omega^2 \qquad \text{(IV.205)}$$

Consequently, it tells us that all constant curvature spaces are *conformally flat*, i.e. related to the flat metric by a conformal factor: $q_k = \Psi_k q_0$. This knowlegde was originally due to Riemann [246, 249–251].
Let us quickly state the range of r': For $k = +1$, we had $r \in [0, 1)$ on which interval the transformations $r \mapsto \tilde{r}(r)$ and $\tilde{r} \mapsto r'(\tilde{r})$ are both invertible, hence we deduce with $2\tan(\arcsin(1)/2) = 2$ readily that $r' \in [0, 2)$. For $k = 0$ the transformation is simply the identity $r \mapsto r'(r) = r$. In the case $k = -1$, using $\tanh(x/2) = (e^x - 1)/(e^x + 1)$ and $\text{arcsinh}(r) = \ln(r + \sqrt{r^2 + 1})$ yields

$$r'(r) = 2\tanh(\frac{1}{2}\text{arcsinh}(r)) = 2\frac{r + \sqrt{1+r^2} - 1}{r + \sqrt{1+r^2} + 1} \underset{r\to\infty}{\to} 2, \qquad r'(r = 0) = 0 \qquad \text{(IV.206)}$$

and due to strict monotony of both functions follows that we compactified the interval $r \in \mathbb{R}_+$ to $r' \in [0, 2)$. For the sake of completeness we write the full spacetime metric in terms of new adapted Cartesian coordinates $x'^i(r', \theta, \phi)$ as in (IV.193):

$$g_k = -dt^2 + a(t)^2 \frac{\delta_{ij} dx'^i dx'^j}{(1 + \frac{k}{4}r'^2)^2} \qquad \text{(IV.207)}$$

IV.D.2 Deparametrisation with scalar field

In order to study the dynamical evolution of a universe described by a Robertson-Walker metric we must implement the Einstein field equation. However, as already discussed before, in order to talk about *evolution* one needs a reference frame, which serves as a clock. A minimal candidate for this is represented by a free massless scalar field ϕ, described by the action

$$S_\phi = \int_{\mathcal{M}} d^4x\, \mathcal{L} = -\int_{\mathcal{M}} d^4x \frac{1}{2}\sqrt{-g} g^{\mu\nu}(\partial_\mu\phi)(\partial_\nu\phi) \qquad \text{(IV.208)}$$

Indeed, this is the massless version of (II.164) where we are using natural units, i.e. $c = 1$ and set $\kappa_\phi = 1$. We expect the galaxy clusters, that are scattered in the known universe, to be spread homogeneously and will demand in the following that $\partial_a\phi = 0$ for $a = 1, 2, 3$. Moreover, when calculating the Euler-Lagrange equation, to which this scalar field must obey in case of a background Robertson-Walker metric, i.e. $g_{00} = -1$, we find

$$0 = -\partial_\mu \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)} + \frac{\partial\mathcal{L}}{\partial\phi} = \ddot{\phi} \qquad \text{(IV.209)}$$

In other words, the velocity of the field is a constant and - assuming it is not vanishing - this implies that the scalar fields serves as good clock by assigning a unique value $\phi(t) = \phi(t, x)$ to each spatial slice σ_t.
As the matter Einstein field equations (IV.43) are consequently obtained by variation of the total action $S = S_{EH} + S_\phi$ we compute the additional part and call it $\kappa T_{\mu\nu}$, with the *energy density tensor*:

$$T_{\mu\nu} = 2\frac{1}{\sqrt{-g}}\frac{\delta S_\phi}{\delta g^{\mu\nu}} = (\partial_\mu\phi)(\partial_\nu\phi) - \frac{1}{2}q_{\mu\nu}g^{\rho\sigma}(\partial_\rho\phi)(\partial_\sigma\phi) = \dot{\phi}^2\delta^{00}_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\dot{\phi}^2 g_{00} =: \rho\delta^{00}_{\mu\nu} + P(g_{\mu\nu} + \delta^{00}_{\mu\nu}) \qquad \text{(IV.210)}$$

where we used (IV.45) and that due to homogeneity we demanded $\partial_a\phi = 0$. We obtain a relation between the newly defined mass density and pressure: $\rho = p = \dot{\phi}^2/2$.
We shall compute the missing Christoffel symbols of the full spacetime metric g_k where we can use our knowledge from the last section regarding $\Gamma(q)$ (IV.199): $(a = a(t))$

$$\Gamma^c_{ab} = \Gamma^c_{ab}(q) = \frac{k}{a^2}x^c g_{ab}, \qquad \Gamma^0_{ab} = \frac{\dot{a}}{a}g_{ab}, \qquad \Gamma^\mu_{0b} = \frac{1}{2}g^{\mu\nu}\partial_0 g_{\nu b} = \frac{\dot{a}}{a}\delta^\mu_b \qquad \text{(IV.211)}$$

and as before

$$R_{00} = -3\partial_0\frac{\dot a}{a} - (\frac{\dot a}{a})^2(\delta^\lambda_\sigma\delta^\sigma_\lambda - \delta^{\sigma\lambda}_{00}) = -3\frac{\ddot a}{a} \tag{IV.212}$$

$$R_{0b} = -2\partial_0\frac{k}{a^2}x^c g_{cb} + 2\partial_c\frac{\dot a}{a}\delta^c_b + 2\frac{\dot a}{a}\delta^\lambda_b\frac{k}{a^2}x^s g_{s\lambda} - 2\frac{k}{a^2}x^\lambda g_{bs}\frac{\dot a}{a}\delta^s_\lambda = 0 \tag{IV.213}$$

$$\begin{aligned} R_{bc} &= \partial_0\frac{\dot a}{a}g_{bc} - 2\partial_{[b}(g_{s]c}x^s\frac{k}{a^2}) - \delta^l_c g_{bl}\frac{\dot a^2}{a^2} + 2\frac{\dot a^2}{a^2}g_{b[c}\delta^s_{s]} + 2\frac{k^2}{a^4}x^l g_{b[c}g_{s]l}x^s = \\ &= (\frac{\ddot a}{a} + \frac{\dot a^2}{a^2})g_{bc} - \frac{k}{a^2}g_{bc}(1-3) + \frac{\dot a^2}{a^2}g_{bc} - 2\frac{k}{a^2}x^s g_{c[b}\delta_{s]j}x^j\frac{k}{1-kr^2} + 2\frac{k^2}{a^4}g_{b[c}g_{s]j}x^s x^j = \\ &= (\ddot a a + 2\dot a^2 + 2k)\frac{g_{bc}}{a^2} - 2\frac{k^2}{a^2}x^s x^j\left(g_{c[b}\delta_{s]j}\frac{1}{1-kr^2} - g_{b[c}\delta_{s]j} - \frac{kr^2}{1-kr^2}g_{b[c}\delta_{s]j}\right) = \frac{\ddot a a + 2\dot a^2 + 2k}{a^2}g_{bc} \end{aligned} \tag{IV.214}$$

From this follows straightforwardly the Ricci scalar: $R = 6(\ddot a a + \dot a^2 + k)/a^2$. With this we can write down (IV.43) explicitly and find for the 00-component:

$$-3\frac{\ddot a}{a} + 3\frac{\ddot a a + \dot a^2 + k}{a^2} = \kappa\rho \qquad \Rightarrow \qquad \frac{\dot a^2 + k}{a^2} = \kappa\rho \tag{IV.215}$$

and similar for the spatial components (where we can drop the non-degenerate g_{ab} by multiplying with its inverse):

$$(-2\frac{\ddot a a}{a^2} - \frac{\dot a^2}{a^2} - \frac{k}{a^2})g_{ab} = \kappa p\, g_{ab} \qquad \Rightarrow \qquad \frac{\ddot a}{a} = -\frac{\kappa}{2}(p + \frac{\rho}{3}) \tag{IV.216}$$

where we reinserted (IV.215). Together, these two equations are known as the *Friedmann equations*. For every initial choice of scalar field (ρ, p) one has a set of ordinary differential equations, determining $a = a(t) = a(t(\phi))$ where we remember that to each coordinate value t we can assign a physical value of our clock, the scalar field ϕ. A prominent consequence of these equations is that given only $\rho \geq 0,\ p \geq 0$ (IV.216) implies that $\ddot a < 0$. In other words, since we are measuring today $\dot a > 0$ due to redshift [252–255] the universe must have been expanding forever and consequently originated from a point where $a = 0$, thus the metric becomes degenerate and the density of matter and the curvature of spacetime was infinite. This singular state has become known as the *Big Bang*.

We will now investigate how the situation presents itself when attacked from the Hamiltonian point of view. This is where the terminology *deparametrisation* stems from, as one can show that in case of an isotropic spacetime the scalar field introduced in (IV.208) continues to serve as a good clock with respect to which evolution is governed by a physical Hamiltonian H_{phys} which is a function involving the original scalar constraint from (IV.113). As a generalisation we consider the case of a non-trivial lapse function N in the Robertson-Walker metric (IV.192).
In the beginning, we must perform a Legendre transformation of the full action $S_{EH} + S_\phi$. While the first part has already been done, the second is

$$\pi_\phi = \frac{\partial\mathcal{L}}{\partial\dot\phi} = -\sqrt{-g}g^{0\mu}(\partial_\mu\phi) = \frac{\sqrt{-g}}{N^2}\dot\phi \;\Rightarrow\; H_\phi = \int_\sigma d^3x\left(\pi_\phi\dot\phi - \mathcal{L}\right) = \int_\sigma d^3x\frac{N}{\sqrt{q}}\frac{\pi_\phi^2}{2} \tag{IV.217}$$

where we used $g^{00} = -N^{-2}$, (IV.56) and that isotropy means $\partial_a\phi = 0$ and $N^a = 0$. Since one of the primary constraints from GR was $\pi := \frac{\partial}{\partial N}S = 0$, implementing its stability analysis yields due to the lapse appearing in H_ϕ the new total scalar constraint, which is bound to vanish:

$$0 = \dot\pi = \{H_\phi + H_{GR}, \pi\} = C_\phi + C = \frac{\pi_\phi^2}{2\sqrt{q}} + C =: C_{tot} \tag{IV.218}$$

This can be solved for $\pi_\phi = H_{phys} := \sqrt{-2\sqrt{q}C}$ in order to fulfil the constraint, $C_{tot}[N] = 0$. This means that ϕ is pure gauge and thus a reduction the extended phase space $(A^I_a, E^a_I, \phi, \pi_\phi)$ is again isomorphic to (A^I_a, E^a_I).[16]
As we are interested in physical observables, $\mathcal{O}$, these should be objects which are not dependant on our choice of coordinate system. As a change of coordinates can be achieved by the means of a diffeomorphism on $\mathcal{M}$,

[16] This could have also been done with a massive scalar field, yielding the additional term $\sqrt{q}\phi^2 m^2/2$. However, upon solving for π_ϕ and declaring it the to be the physical Hamiltonian $p_\phi =: H_{phys}(\phi)$ this objects depends on the clock, i.e. dynamics is governed by a time-dependent Hamiltonian. To keep the analysis simpler we do not include any potential.

especially the diffeomorphism associated with Nn (see theorem IV.B.2) should leave the observable invariant, i.e. $\mathcal{L}_{Nn}\mathcal{O} = 0$ by definition IV.A.8. It can be shown that the generator of these diffeomorphism equals

$$\mathcal{L}_{Nn}\mathcal{O} = \{C_{tot}[N], \mathcal{O}\} = 0 \tag{IV.219}$$

In other words this is a gauge freedom and the observable $\mathcal{O}$ should not depend on this gauge.
In order to impose (IV.219) we will first choose a specific lapse function. Note that this choice does not change the dynamics of the theory under consideration, as it corresponds merely to a change of the coordinate time. A convenient choice is $N = V$, which implies $C_{tot}[N] = \int_\sigma (\pi_\phi^2 - 2\sqrt{q}H_{phys})$. Now we can use (IV.219) to find the evolution of $\mathcal{O}(\phi)$ with respect to the clock field ϕ. Similar constructions can also be carried out with other forms of matter, but since we only wanted to give a proof of principle we refer for those approaches to the literature [147–153].
The problem to understand the evolution of observables related to our system (e.g. the volume of the isotropic universe, which can be expressed as (IV.114)) reduce hence to expressing C in terms of the Ashtekar-Barbero variables. (IV.207) is already given in a form from which we can easily read off lapse, shift and spatial metric as expressed in (IV.50):

$$N = 1, \qquad N^a = 0, \qquad q_{ab} = a(t)^2 z_{r'}^{-2}\delta_{ab} \tag{IV.220}$$

with $z_{r'} := 1 + kr'^2/4$. Since q_{ab} is in a diagonal form, it is easy to define the co-3-bein e_a^I and its inverse:

$$e_a^I = \frac{a}{z_{r'}}\delta_a^I, \qquad e_I^a = \frac{z_{r'}}{a}\delta_I^a \tag{IV.221}$$

Due to the appearance of δ_a^I the computation for the spin-connection gets hugely simplified, as well as for the extrinsic curvature (remember $e_I^b e_b^J = \delta_I^J$)

$$K_{ab} = \frac{1}{2N}\dot{q}_{ab} = \frac{\dot{a}}{Na}q_{ab} =: \frac{c}{\beta a}e_a^I \delta_{IJ} e_b^J \tag{IV.222}$$

$$\begin{aligned}\Gamma_a^L &= -\frac{1}{2}\epsilon^{LJK}e_K^b\left(2\partial_{[b}e_{a]}^J + e_J^c e_a^M \partial_b e_c^M\right) = \\ &= -\frac{1}{2}\epsilon^{LJb}z_{r'}\left(\delta_a^J\frac{-k}{4z_{r'}}2\delta_{bj}x'^j - 0 + \delta_a^J\frac{-k}{4z_{r'}}2\delta_{bj}x'^j\right) = \frac{k}{2}\epsilon_{Laj}x'^j z_{r'}^{-1}\end{aligned} \tag{IV.223}$$

which gives us for the connection and the electric field:

$$E_I^a = |\det(\{e_b^J\}_b^J)|\, e_I^a = a^2 z_{r'}^{-2}\,\delta_I^a =: p z_{r'}^{-2}\,\delta_I^a \qquad A_a^I = \Gamma_a^I + \beta K_{ab}e_I^b =: z_{r'}^{-1}(\frac{k}{2}\epsilon_{Iaj}x'^j + c\,\delta_a^I) \tag{IV.224}$$

Consequently, the whole kinematical information of the phase-space of an isotropic spacetime with constant curvature k can be described by the pair (c, p).
It is easily verified that this solution satisfies the Gauss constraint:

$$G_J = \partial_a E_J^a + \epsilon_{JKL}A_a^K E_L^a = \frac{pk}{2z_{r'}^3}\left(-2x'^J + x'^I\epsilon_{JKa}\epsilon^{KaI}\right) = 0 \tag{IV.225}$$

For (IV.113), the scalar constraint, note that the Poisson brackets must be evaluated via (IV.117) and (IV.118) before plugging in (IV.224):

$$\begin{aligned}C_E &= \frac{1}{\kappa}F_{ab}^J\epsilon_{JKL}\frac{E_K^a E_L^b}{\sqrt{\det(E)}} = \frac{\sqrt{p}}{\kappa}z_{r'}^{-1}\left(2\partial_{[a}A_{b]}^J\epsilon^{Jab} + 2A_a^{[a}A_b^{b]}\right) = \\ &= \frac{\sqrt{p}}{\kappa z_{r'}^3}\left(z_{r'}k\epsilon_{J[ba]}\epsilon^{Jab} - \frac{k^2}{4}2x'^i\delta_{i[a}\epsilon_{b]jJ}x'^j\epsilon^{Jab} + 9c^2 - 3c^2 - \frac{k^2}{4}\epsilon_{abj}x'^j\epsilon^{ba}{}_i x'^i\right) = \\ &= \frac{\sqrt{p}}{\kappa z_{r'}^3}\left(-6k - \frac{6k^2}{4}r'^2 + 6c^2 + k^2r'^2 + \frac{1}{2}k^2r'^2\right) = \frac{6\sqrt{p}}{\kappa z_{r'}^3}(-k + c^2)\end{aligned} \tag{IV.226}$$

$$C - C_E = -\frac{1+\beta^2}{\kappa}\epsilon_{JMN}K_a^M K_b^N\epsilon_{JKL}\frac{E_K^a E_L^b}{\sqrt{\det(E)}} = -\frac{1+\beta^2}{\beta^2}\frac{6\sqrt{p}}{\kappa z_{r'}^3}c^2 \tag{IV.227}$$

One can extract several physically interesting observations from these expressions. For example, upon recalling (IV.129) and the first line of (IV.130) we see that

$$\beta^2 C + C_E = \frac{\sqrt{q}}{\kappa}\left(\beta^2(-R^{(3)} + K_{ab}K^{ab} - K^2) + (-R^{(3)} - \beta^2(K_{ab}K^{ab} - K^2))\right) = -(1+\beta^2)\frac{\sqrt{q}}{\kappa}R^{(3)} \tag{IV.228}$$

and hence in case of isotropy we get explicitly:

$$\beta^2 C + C_E = \frac{6\sqrt{p}}{\kappa z_{r'}^3}\left(-(1+\beta^2)c^2 + (1-\beta^2)(-k+c^2)\right) = -(1+\beta^2)\frac{\sqrt{q}}{p\kappa}6k \tag{IV.229}$$

which with $a^2 = p$ yield together $R = 6k/a^2$, which is in agreement with (IV.203).
Similarly, using (IV.218) we find the total physical Hamiltonian of our system to be:

$$H_{phys} = \sqrt{-2\sqrt{q}C} = \left(\frac{12}{\kappa}\frac{p^2}{z_{r'}^6}(c^2/\beta^2 + k)\right)^{1/2} = \sqrt{\frac{12}{\kappa}}(1+\frac{k}{4}r'^2)^{-3}a^2\sqrt{\dot{a}^2/N^2 + k} \tag{IV.230}$$

One can perform a symplectic reduction: Let f_1, f_2 be two functions on the phase space spanned by $(A_a^I = c\delta_a^I, E_J^b = p\delta_J^b)$ and X_{f_i} the Hamiltonian flow generated by f_i. The Poisson bracket between f_1, f_2 can be rewritten as the symplectic form $dE_I^a \wedge dA_a^I$ evaluated on the X_{f_i} and hence:

$$\{f_1, f_2\}_{E,A} = \int_\sigma d^3x \frac{\delta f_{[1}}{\delta E_I^a}\frac{\delta f_{2]}}{\delta A_a^I} = (\int_\sigma dE_I^a \wedge dA_a^I)(X_{f_1}, X_{f_2}) = \tag{IV.231}$$

$$= (\int_\sigma \delta_I^a dp \wedge z_{r'}^{-1}(\frac{k}{2}\epsilon_{Iaj}dx'^j + \delta_a^I dc))(X_{f_1}, X_{f_2}) = (\delta_I^I dp \wedge dc \int_\sigma z_{r'}^{-1})(X_{f_1}, X_{f_2}) = \tag{IV.232}$$

$$= 3V_0\{f_1, f_2\}_{p,c}$$

with the formal definition $V_0 := \int_\sigma d^3x' z_{r'}^{-1}$. We can deduce that this induces the Poisson bracket $\{p, c\} = \frac{\kappa\beta}{6V_0}$.
Choosing the scale factor $a(t(\phi))^2 = p$ as observable ,which depends on time (the clock ϕ), we can compute its time evolution . This yields an exponential expansion of the scale factor, which also deploys the same initial Big Bang singularity as does the Friedmann equation.

IV.D.3 Classical Discretisation Ambiguities

In this paragraph we will investigate the subtleties arising, when one introduces e.g. a cubulation $T(\epsilon)$ of the spatial slice σ with respect to some parameter ϵ. We will see that even on the classical level the Hamiltonian picks up an arbitrariness that can only be resolved when taking the continuum limit, i.e. $\epsilon \to 0$.
In Corollary IV.C.2 we already presented *one* possible way to regularise the scalar constraint of GR, by $C = C^\epsilon + \mathcal{O}(\epsilon)$. To provide a concrete example, we will show how this purely classical discretisation reads for our isotropic model (IV.226,IV.227). In order to do so, we have to compute the holonomies along the curves $e_{p,i}$ of a chosen cubulation. Here we will pick a family of cubic lattices (labelled by ϵ), so that their axes can be oriented along a fiducial Cartesian system of coordinates of the 3-geometry, defined by $dx'^{|i|}$.[17] Further, we restrict to an artificial model on the compact spatial manifold $\sigma = T^3$, i.e. the three torus. This is reminiscent to the $k = 0$ model of an FRLW universe, with the exception of having a finite volume $V < \infty$. The edges $e_{p,i}(t)$ are labelled by their starting point p, a vertex on the lattice, and the direction $i \in \{\pm1, \pm2, \pm3\}$ along which they leave p with $\dot{e}_{p,i}^a(t) = sgn(i)\delta_{|i|}^a$. Along this curve the value $\epsilon_{|i|aj}x'^j(e_{p,i})$ remains constant and hence all matrices $A_a(e_{p,i}(t))$ for all t in the same edge $e_{p,i}$ commute with each other. Although the computation could also be done in a lengthy way for $k = \pm1$, for sake of brevity we will stick to the flat metric in the following.
Since $z_{r'} = 1$ and (IV.224) reduces to $E_I^a = p\delta_I^a$ and $A_a^I = c\delta_a^I$ we find for (IV.154), using that each τ_I commutes with itself, $(I := |i|)$

$$h_\epsilon(e_{p,i}) = \mathcal{P}\exp(\int_0^\epsilon ds\ \dot{e}_{p,i}^a A_a^J(e_{p,i}(t))\tau_J) = \exp(sgn(i)c\epsilon\tau_I) \tag{IV.233}$$

Using (IV.141) we can compute the curvature which by (IV.175) can be written as the holonomy along a closed path, for which we choose a small rectangle in the $i - j$ plane:

$$\begin{aligned} h(\Box_{ij}^\epsilon) &= e^{sgn(i)\epsilon c\tau_I}e^{sgn(j)\epsilon c\tau_J}e^{-sgn(i)\epsilon c\tau_I}e^{-sgn(j)\epsilon c\tau_J} = \\ &= \mathbb{1}_2 + e^{sgn(i)\epsilon c\tau_I}e^{sgn(j)\epsilon c\tau_J}[e^{-sgn(i)\epsilon c\tau_I}, e^{-sgn(j)\epsilon c\tau_J}] = \\ &= \mathbb{1}_2 + e^{sgn(i)\epsilon c\tau_I}e^{sgn(j)\epsilon c\tau_J}\ 4sgn(ij)\sin(\frac{\epsilon c}{2})^2\epsilon_{IJK}\tau_K \end{aligned} \tag{IV.234}$$

[17] As the lattice family is only an intermediate object of no physical relevance, this choice is arbitrary, as long as all cells of its dual complex are of vanishing volume for $\epsilon \to 0$.

and with $\tau_I\tau_J = -\delta_{IJ}/4 + \epsilon_{IJK}\tau_K$, $\tau_I\tau_J + \tau_J\tau_I = 0$ and $h(e)^\dagger = h(e^{-1})$: (no sum over I, J)

$$\begin{aligned}
h(\Box^\epsilon_{ij}) - h(\Box^\epsilon_{ji}) &= 4\sin(\frac{\epsilon c}{2})^2 \Big(2sgn(ij)\cos(\frac{\epsilon c}{2})^2\epsilon_{[IJ]K}\tau_K + 2\sin(\frac{\epsilon c}{2})^2\tau_{[I}\tau_{J]}\epsilon_{IJK}\tau_K \\
&\quad + \sin(\frac{\epsilon c}{2})\cos(\frac{\epsilon c}{2})(sgn(j)\tau_I + sgn(i)\tau_J + sgn(i)\tau_J + sgn(j)\tau_I)\epsilon_{IJK}\tau_K\Big) \\
&= 2sgn(ij)\sin(\epsilon c)^2\epsilon_{IJK}\tau_K + 2^5\sin(\frac{\epsilon c}{2})^4\mathbb{1}_2
\end{aligned} \tag{IV.235}$$

Now using that $\sum_{i,j}\epsilon(i,j,k)sgn(ijk)\epsilon_{|i||j|K} = 8\delta_{|k|K}$ and $T_v = 2^3$ we find for (IV.183)

$$\begin{aligned}
C^\epsilon_E &= \frac{-4}{\kappa^2\beta T_v}\epsilon(i,j,k)tr\left((h(\Box^\epsilon_{ij}) - h(\Box^\epsilon_{ji})h(e_k)\{h(e_k^{-1}), V_\epsilon\}\right) = \\
&= \frac{-4}{\kappa^2\beta T_v}\epsilon(i,j,k)2sgn(ij)\sin(\epsilon c)^2\epsilon_{IJK}tr(\tau_K\tau_{|k|})(-sgn(k)\epsilon)\{c,p\}\frac{3}{2}\sqrt{p}V_0 = \\
&= \frac{1}{\kappa T_v}48\epsilon\sqrt{p}\sin(\epsilon c)^2 = \frac{6\epsilon^3}{\kappa}\sqrt{p}\frac{\sin(\epsilon c)^2}{\epsilon^2}
\end{aligned} \tag{IV.236}$$

where we have chosen $V_\epsilon = V$ and used $\{p,c\} = \kappa\beta/(6V_0)$. With this we see that indeed we recover the known expression in the continuum limit:

$$C^\epsilon_E[1] = \sum_v \epsilon^3 C^\epsilon_E \underset{\epsilon\to 0}{\longrightarrow} \int_\sigma d^3x\ \frac{6}{\kappa}\sqrt{p}\frac{\sin(\epsilon c)^2}{\epsilon^2} = C_E(1) \tag{IV.237}$$

where we used that σ is completely triangulated with cells of coordinate volume ϵ^3. Assuming a compact spatial manifold gives thus $\sum_v \epsilon^3 = \frac{V_0}{\epsilon^3}\epsilon^3 = V_0$. With this we see also:

$$\{C^\epsilon_E[1], V\} = \frac{6}{\kappa}V_0^2\frac{3}{2}\sqrt{p}\{\frac{\sin(\epsilon c)^2}{\epsilon^2}, p\} = -\frac{3\beta}{2}V_0 p\frac{\sin(2\epsilon c)}{\epsilon} \tag{IV.238}$$

And thus for the full scalar constraint (IV.182):

$$\begin{aligned}
C^\epsilon &= C^\epsilon_E + \frac{4^3(1+\beta^2)}{\kappa^4\beta^7}\frac{\epsilon(i,j,k)}{T_v}tr(\{sgn(i)\epsilon c, \{C^\epsilon_E, V\}\}\{sgn(j)\epsilon c, \{C^\epsilon_E, V\}\}\{sgn(k)\epsilon c, V\}) = \\
&= C^\epsilon_E + \frac{4^3(1+\beta^2)}{\kappa^4\beta^7}\frac{1}{T_v}\epsilon^3\left(\frac{3\beta}{2}V_0\frac{\sin(2\epsilon c)}{\epsilon}\{c,p\}\right)^2 V_0\sqrt{p}\frac{3}{2}\{c,p\}tr(8\epsilon_{IJK}\tau_I\tau_J\tau_K) = \\
&= C^\epsilon_E - \frac{1+\beta^2}{\kappa\beta^2}\frac{2}{T_v}6\frac{\sin(2\epsilon c)^2}{\epsilon^2}\sqrt{p}\epsilon^3 = \frac{6\epsilon^3}{\kappa}\sqrt{p}\left(\frac{\sin(\epsilon c)^2}{\epsilon^2} - \frac{1+\beta^2}{\beta^2}\frac{\sin(2\epsilon c)^2}{4\epsilon^2}\right)
\end{aligned} \tag{IV.239}$$

Again the continuum limit $\epsilon \to 0$ yields the correct result. It is worthwhile to point out that due to (IV.229) we know that $\beta^2 C + C_E \sim R^{(3)} = 0$, however $\beta^2 C^\epsilon + C^\epsilon_E = \mathcal{O}(\epsilon)$. Thus, while recovering the correct expression for $\epsilon \to 0$, we see that for finite ϵ the theory is *not* capturing isotropic flat spacetime. In fact, this has quite drastic influence on the evolution of observables, such as the volume of the spatial slice. See figure IV.1 for further details.

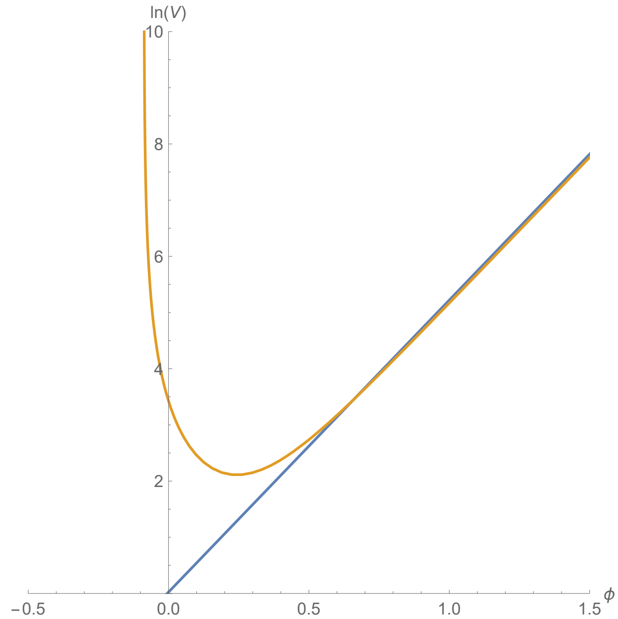

Abbildung IV.1: Plot of the Volume $V = p^{3/2}$ of the compact spatial slice $\sigma = [0,1)^3$ reminiscent of the flat FRLW model for our universe against the physical time ϕ, i.e. the clock field. ($\beta = \kappa = 1$, $\phi(t=0) = 0.66$). In blue, the classical trajectory governed by the Hamiltonian (IV.226) & (IV.227) is plotted, where the universe stems from a singularity at $\phi = 0$. In orange, a naive *discretisation* (IV.239) has been used to compute the dynamics. While in agreement at late times, $\phi >> 1$, the lattice effects are significant in the early universe and even predict the replacement of the singularity with an asymmetrical "Big Bounce". However, as of today it is up to discussion, whether the details of this old, contracting universe are really physical.

We want to finish this chapter with an even stronger disclaimer of why the corrections obtained in (IV.239) are probably not supposed to give rise to physical predictions.
Consider $Z \in \mathbb{N}_+$ with $Z < \infty$. Then there exists a $\mathcal{N} = \mathcal{N}(Z) \in \mathbb{N}$ such that $\mathcal{N}(Z) < \infty$ and one finds solution $\{g_n\}_{n\in\{1..\mathcal{N}\}}$ of

$$\sum_{n=1}^{\mathcal{N}} g_n n = 1, \qquad \sum_{n=1}^{\mathcal{N}} g_n n^i = 0 \quad \forall i \ : \ 2 \leq i \leq Z \tag{IV.240}$$

Let us call $g_0 := \sum_{n=1}^{\mathcal{N}} g_n$. Then define the following set of curves: For $n \in \{1...\mathcal{N}\}$ we choose ${}^n e(t)$ such that ${}^n\dot{e}(t)^a = \delta^a_i n$ and ${}^n e(t=0) = x$ (without loss of generality we set in the following $x = 0$). Furthermore we call ${}^n e_\epsilon(t) := {}^n e(t\epsilon)$. Then we see (using linearity to exchange a finite with an infinite sum)

$$\begin{aligned}
\sum_{n=1}^{\mathcal{N}} g_n h({}^n e_\epsilon) - \mathbb{1}_2 g_0 &= \sum_{n=1}^{\mathcal{N}} g_n \sum_{k=1}^{\infty} \int_0^1 dt_1 \, ... \int_0^{t_{k-1}} dt_k \; a_e(t_k)...A_e(t_1) = \\
&= \sum_{n=1}^{\mathcal{N}} g_N \sum_{k=1}^{\infty} \int ... \int (n\epsilon\delta^a_i A_a({}^n e_\epsilon(t_k)) ... = \sum_{n=1}^{\mathcal{N}} g_n \sum_{k=1}^{\infty} \int ... \int (n\epsilon)^k \sum_{l_1} (n\epsilon)^{l_1} \frac{1}{l_1!} \partial^{(l_1)} A_i(0)... \\
&= \sum_{k=1}^{\infty} \sum_{l_1..l_k} \left(\sum_{n=1}^{\mathcal{N}} g_n n^{k+\sum l_i} \right) \epsilon^{k+\sum l_i} \frac{1}{l_1!...l_k!} \partial^{(l_1)} A_i(0)..\partial^{(l_k)} A_i(0) = \epsilon A_e(0) + \mathcal{O}(\epsilon^{Z+1})
\end{aligned} \tag{IV.241}$$

In other words, we have significantly improved the approximation (IV.173) in the Non-Abelian Stokes theorem. By the same calculation one also gets:

$$\sum_{n=1}^{\mathcal{N}} g_n h({}^n e_\epsilon)\{h({}^n e_\epsilon)^\dagger, V\} = \{A_i(x), V\} + \mathcal{O}(\epsilon^{Z+1}) \tag{IV.242}$$

$$\frac{1}{2\epsilon^2} \sum_{m=1}^{\mathcal{N}'} g'_m (h({}^m\Box^\epsilon_{x,uv}) - h({}^m\Box^\epsilon_{x,uv})^{-1}) = u^a v^b F_{ab}(x) + \mathcal{O}(\epsilon^{Z+1}) \tag{IV.243}$$

for coefficients g'_m such that $\sum_{m=1}^{\mathcal{N}'} m^i g'_m = \delta(2,i)$ for $i \leq Z$. Hence for any $Z \in \mathbb{N}$ we can construct a regularisation along the lines of corollary IV.C.2 as

$$\begin{aligned} {}^Z C^\epsilon := {}^Z C_E^\epsilon + \frac{4^3(1+\beta^2)}{\kappa^4\beta^7}\sum_{ijk}\frac{\epsilon(i,j,k)}{T_v}\sum_{n,m,l}^{\mathcal{N}} g_n g_m g_l \times \\ \times tr\left(h({}^n e_i)\{h({}^n e_i)^\dagger, \{V, {}^Z C_E^\epsilon[1]\}\}h({}^m e_j)\{h^\dagger({}^m e_j), \{V, {}^Z C_E^\epsilon[1]\}\}h({}^l e_k)\{h^\dagger({}^l e_k), V_\epsilon(v)\}\right) \end{aligned} \tag{IV.244}$$

$${}^Z C_E^\epsilon := \frac{-4}{\kappa^2\beta}\sum_{ijk}\frac{\epsilon(i,j,k)}{T_v}\sum_n^{\mathcal{N}}\sum_m^{\mathcal{N}'} g_n g'_m tr\left((h({}^n\Box_{v,ij}^\epsilon) - h^\dagger({}^n\Box_{v,ij}^\epsilon))h({}^m e_k)\{h^\dagger({}^m e_k), V_\epsilon(v)\}\right) \tag{IV.245}$$

Going with this through the computation (IV.236) yields

$${}^Z C_E^\epsilon = \epsilon\frac{6\sqrt{p}}{\kappa}\sum_n g_n n\left(\sum_m g'_m \sin(m\epsilon c)^2\right) = \epsilon\frac{6\sqrt{p}}{\kappa}\left(\sum_m g'_m \sin(m\epsilon c)^2\right) + \mathcal{O}(\epsilon^{Z+1}) \tag{IV.246}$$

where the bracket term will also be $c^2 + \mathcal{O}(\epsilon^{Z+1})$. Also we get

$${}^Z C^\epsilon - {}^Z C_E^\epsilon = -\frac{1+\beta^2}{\kappa\beta}6\epsilon^3\sqrt{p}\left(\sum_m g'_m \, m \, \frac{\sin(2m\epsilon c)}{2\epsilon}\right)^2 \tag{IV.247}$$

from which the reader can deduce that again no corrections lower than ϵ^{Z+1} remain.
The main message we want to communicate with this example is that e.g. a quantum theory of isotropic cosmology built on an arbitrary regularisation like (IV.239) is not expected to make any reliable physical predictions as soon as the phase space variables (p, c) reach the order of magnitude of the regularisation parameter ϵ, as is the case once one approaches the Big Bang singularity.

Hence, the effect of these ambiguities and the task to find reliable discretised dynamics must not be neglected, once a finite lattice is used in an intermediate step. This problem is of grave importance in the context of quantum field theories. As we discussed in chapter *III. Renormalisation*, it might be possible that a cylindrically consistent fixed point describes the correct dynamical predictions of a theory of Quantum Gravity.

Kapitel V

Loop Quantum Gravity

One of the major unresolved problems of foundational physics is to find a consistent theory of Quantum Gravity (QG). For more than 80 years, physicists have tried to tackle this problem, yet a completely satisfying answer has not been found as of today. But without a reliable quantisation of GR we fall short in explaining the limits of Einstein's famous theory, e.g. the Big Bang singularity.
In this chapter, we will study one of the most prominent approaches towards this theory, namely *Loop Quantum Gravity* (LQG). This is a mathematically rigorous, non-perturbative and background independent quantum field theory developed in the spirit of constructive QFT as discussed in chapter *II. Quantum Field Theory*. The so-called Dirac programme [42–45] of canonical quantisation has been expanded by various authors to background independent representations [201–205, 256, 257]. We will briefly state the stages of this programme in the way they appear in LQG and by this make contact with what has been said earlier about the construction of quantum field theories. The novelty in this case comes from the presence of non-trivial constraints. E.g. instead of a Hamiltonian generating time evolution we have to deal with the scalar constraint. In other words, we cannot use the first one to single out a vacuum vector. The Dirac programme in LQG reads:[1]

1 The holonomies $h(e) \in \mathrm{SU}(2)$ and fluxes $E(S) \in \mathfrak{su}(2)$ for all piecewise analytic edges e and surfaces S built from the Ashtekar-Barbero variables are chosen as the elements of $\mathcal{E}$. On those, the standard commutation relations are implemented in terms of a non-commutative product, i.e. $\{.,.\} \to -i/\hbar\,[.,.]$.

2 Afterwards, one has to pick a state ω on the algebra of observables $\mathcal{A}$ (generated from $\mathcal{E}$). As we saw, this is related to finding a representation of the phase space variables of the theory, as operators in an auxiliary Hilbert space $\mathcal{H}_{kin}$ and a suitable vacuum vector. To single out one of the many choices, we impose the physical sensible restriction for the state to be *diffeomorphism-invariant*.

3 Additionally, the constraints have to be promoted to (self-adjoint) operators in $\mathcal{H}_{kin}$. In the case of GR, these are the Gauss constraint G_J, the diffeomorphism constraint $\vec{C}$ and the scalar constraint C.

4a Characterise the space of solutions of the constraints $G_J, \vec{C}$ and define the corresponding inner product that defines the Hilbert space $\mathcal{H} \subset \mathcal{H}_{kin}$. Now, one can continue in this direction and also solves the scalar constraint to define the physical Hilbert space $\mathcal{H}_{phys} \subset \mathcal{H}$.

4b Alternatively, after constructing $\mathcal{H}$, the space on which the constraints $G_J, \vec{C}$ are solved, we invoke the concept of *deparametrisation*. We remember from *IV General Relativity* that for example dust fields can be used as clocks with respect to which (a part of) the scalar constraint becomes a *true Hamiltonian* which generates time-translations. We then promote it to a self-adjoint operator and study the evolution with respect to the clock field.

5 Find a (complete) set of gauge invariant observables, i.e. operators commuting with the constraints. They represent the physical experiments whose outcomes our quantum theory can predict.

In the following sections we will undergo the first three steps of this construction. When implementing the scalar constraint, we will find it is highly prone to different choices of regularisation. Hence, without renormalising our theory as described in chapter *III. Renormalisation*, we should not continue with the programme of canonical quantisation.

[1] Here, we state it explicitly in the version where the constraints are promoted to operators on the Hilbert space. There is an alternative programme, where the constraints are already solved at the classical level.

The first question we must address is why we choose the holonomy-flux algebra from among the many possibilities to describe the theory of GR. As we remember, the phase space of GR was coordinatised by the connection field $A^I_a(x)$ and its canonical conjugated momentum $E^b_J(y)$ which had the non-vanishing Poisson-bracket

$$\{ A^I_a(x) \, , \, E^b_J(y) \} \; = \; \frac{\kappa\beta}{2} \, \delta^{(3)}(x,y) \tag{V.1}$$

containing the Dirac δ distribution and the Immirzi parameter $\beta \neq 0$. In order to promote this into a relation between operators (rather than operator-valued distributions) we must smear it with background independent test functions. While for this aim a lot of smearings are possible, we want to choose one which behaves especially nice under gauge transformations. This is the aforementioned holonomy-flux algebra, which for GR has been considered mathematically precise for the first time in [258]. From the experience gained in non-abelian Yang-Mills theories, we choose fluxes smeared in two dimensions and, instead of the connection, the path-ordered exponentials of A^I_a along some curves. These are exponentials of Lie algebra elements and as such $\mathrm{SU}(2)$-valued. This puts us moreover in the advantageous position that we can use the Peter & Weyl theorem (see theorem II.A.5), which tells us how a Hilbert space over a compact gauge group can be constructed.
Thus, it is the holonomy-flux algebra which will be considered in *V.A. Kinematical Hilbert space of LQG* as subset $\mathcal{E}$ for which we want to develop a quantum theory. Then, we replace its product by a non-commutative version to generate $\hat{\mathcal{A}}$. With every polynomial function in the holonomies and fluxes we can associated a graph γ, say $F_\gamma \in \hat{\mathcal{A}}$. γ is such that in $E(\gamma)$, i.e. the edges of γ, we find an edge for every holonomy in F_γ.
The next step is then the choice of a corresponding state. In the first chapters we saw that a lot of ambiguities arose due to the many inequivalent irreducible representations of $\hat{\mathcal{A}}$. However, in LQG the situation can be significantly improved by demanding that the state shall be diffeomorphism-invariant. A state satisfying this criterion is the *Ashtekar-Isham-Lewandowski state* ω_{AL} [66] reading explicitly on $\hat{\mathcal{A}}$

$$\omega_{AL}\Big(\; F(\{h(e_I)\}_I \;) \, \star \hat{E}_{f_1}(S_1) \star ... \star \hat{E}_{f_N}(S_N) \; \Big) \; = \; \begin{cases} 0 & \text{if } N > 0 \\ \mu_H(F) & \text{else} \end{cases} \tag{V.2}$$

where μ_H is the Haar measure over several copies of $\mathrm{SU}(2)$ on the graph with which $F = F_\gamma$ can be associated [67, 259–262]:

$$\mu_H(F) = \int_{\mathrm{SU}(2)^{|E(\gamma)|}} \prod_{e \in E(\gamma)} d\mu_H(g_e) F_\gamma(\{g_e\}_e) \tag{V.3}$$

The state ω_{AL} serves as a candidate for a vacuum in the algebraical sense, by being a state where no metric degrees of freedom have been excited.[2] There is a uniqueness theorem [68], which tells us that ω_{AL} is indeed the *only* possible state, that is diffeomorphism-invariant (and satisfies certain regularity assumptions) [69–73]. For this reason, the state serves as the starting point for all further considerations.
We can also consider the GNS construction of this state, in order to obtain a Hilbert space $\mathcal{H}_{kin}$ and a representation of the algebra as operators thereon. The corresponding GNS vector to ω_{AL} is the vacuum vector Ω_{AL}. We define holonomy and flux operators $\hat{h}_{ab}(e)$ and $\hat{E}(S)$ on $\mathcal{H}_{kin}$ which is the Cauchy completion of the span of all cylindrical functions over all finite graphs. By a finite graph γ we understand a finite collection of curves $\{e_I\}_I$ meeting at their end points at most. E.g., $\mathcal{H}_\gamma \subset \mathcal{H}_{kin}$ is the completion of the span of polynomial functions of the holonomy operators $\hat{h}(e)$, $e \in E(\gamma)$ applied to Ω_{AL}.[3] Note that Ω_{AL} is annihilated by all $\hat{E}(S)$.
Thus, approximations to all possible geometries are supposed to be constructed from Ω_{AL} by suitable actions of holonomy operators on it, a property because of which we call it *cyclic*. A geometry in which we are especially interested to construct is one, by which the universe appears manifestly classical. A vector in $\mathcal{H}_{kin}$ resembling this feature must be such that if we compute the expectation value of some observables, e.g. a holonomy along a curve e, we are to obtain the classical value plus small corrections. If this is the case for all observables we are interested in, we call it a *coherent state*. We will repeat the explicit construction of gauge coherent states from [154–158, 263, 264]. Notably, they can be peaked on the classical variables of a holonomy along a curve and on the flux through a surface associated with the mentioned curve. By representing what could be called "Gaussian wavepackets" on the group $\mathrm{SU}(2)$, they are labelled by their spread, $t \in \mathbb{R}_+$, which

[2] One should not confuse this with a state describing an empty, i.e. flat universe, which comes equipped with the Minkowski metric. Rather, this state corresponds to a state where "no space exists", e.g. the expectation value for the volume of any region vanishes.

[3] Albeit its innocent looking definition, this Hilbert space turns out to be non-separable due to the huge number of possible graphs.

we will typically choose to be of order $\hbar$. Later on, we will use this concept by choosing special coherent states which are peaked over a classical flat Robertson-Walker spacetime and use them to compute the expectation values of certain observables.

This, in return, means that we first have to understand how classical observables are quantised in the context of LQG. We will repeat this in *V.B. Quantisation of Geometric Operators and Constraints*.
Since GR is a theory about geometry, its pivotal operators are those describing geometric quantities. Foremost, the volume of certain regions is an object used in many other constructions, such as the scalar constraint. As its classical expression was the square root over the determinant of the metric integrated over a region B, a straightforward quantisation on $\mathcal{H}_\gamma$ is the one proposed by Ashtekar and Lewandowski in [266], i.e.

$$\hat{V}_{AL}(B) := \frac{(\beta\hbar\kappa)^{3/2}}{2^5\sqrt{3}} \sum_{v\in V(\gamma)} \sqrt{|\hat{Q}_v|}, \qquad \text{(V.4)}$$
$$\hat{Q}_v := i \sum_{e\cap e'\cap e''=v} sgn(\det(\dot{e},\dot{e}',\dot{e}''))\epsilon_{IJK}\hat{E}^I(S_e)\hat{E}^J(S_{e'})\hat{E}^K(S_{e''})$$

where $V(\gamma)$ is the set of points where at least three edges meet. The three edges e, e', e'' are all incident, i.e. share the vertex v as starting point, and we associate a suitable surface S_e to each of them, which will be infinitesimal close to the vertex.[4] One should note that the square root in the definition of (V.4) is to be understood in the sense of the spectral theorem. Hence, we must first diagonalise the operator $\hat{Q}_v$ on a given graph Hilbert space, before we can fully understand the action of the Ashtekar-Lewandowski volume. This fact makes the analysis of many quantities very hard and only partial results have been achieved so far, e.g. the matrix elements of $\hat{Q}_v$ are known [270] and some advances in the spectral analysis of the volume operator can be found in [271–273].
We like to point out that the situation is vastly different for another geometric operator, namely the area operator [265]. Following the same strategy as for the volume, one obtains upon quantisation an operator whose action on a given graph can be easily computed. It turns out, that its spectrum is discrete and bounded from below, with minimal non-vanishing eigenvalue Δ. The interpretation of this would be that there is a minimal area which can be measured during an experiment, and later we will see how this fact has been used for defining symmetry reduced models for quantum cosmology.
Also, one was able to implement the Gauss und the diffeomorphism constraints properly. The first one can be solved in numerous equivalent ways, leading to the subspace of $\mathcal{H}$, called $\mathcal{H}_G$ which is the span of the (gauge-invariant) *spin-network functions* [274–278]. In contrast to this, the implementation of the diffeomorphism constraint is normally achieved via *group averaging* with respect to (a generalisation of) the spatial diffeomorphism group $\mathrm{Diff}(\sigma)$.
The most complicated object to deal with, however, is the scalar constraint. By choosing the corresponding element in $\hat{\mathcal{A}}$, such that the volume operator appears on the right, the scalar constraint is automatically annihilating the vacuum vector Ω_{AL}. (In the presence of appropriate dust fields, the constraint can be associated with a physical Hamiltonian, which has the same property.) We already saw in the last chapter that there exists an approximation, C^ϵ, of the scalar constraint using holonomies along loops of coordinate length 4ϵ. In [74, 75] it was hence proposed to regularise the action of $\hat{C}^\epsilon$ on the vertex v of a finite graph γ (whose edges will not be infinitesimally short) by adding infinitesimal loops between edges incident at v. This finishes the full description of a continuum quantum theory of GR.
However, as we could see in the chapter about renormalisation, as soon as one introduces a regularisation, one has to ask whether there are ambiguities which lead to different physical predictions. Another possible, yet arbitrary alternative to the *Thiemann regularisation* mentioned above was introduced in [279–281], where the structure of the scalar constraint was considerably changed. As it turns out, both regularisations agree only in the continuum limit before quantisation. Due to the involved action, it has been difficult to investigate the difference in these (and other possible) regularisations at the quantum level.

A possible strategy to solve these problems presents itself, when trying to regularise the system in a non graph-changing way: From the philosophy advocated earlier, this corresponds to considering a given graph γ (which shall be such that it could be used to give rise a dual cell complex of σ) as a possible discretisation of the system and studying the projection of all observables on the mentioned coarse resolution. The first incarnation of this approach is called *Algebraic Quantum Gravity* in [92–95].[5] Here, one takes an infinite graph which

[4] It is worthwhile to note that there are also other proposals for volume operators in the literature, e.g. in [267]. However, the quantisation given in the main body of the text is as of today the only one, which is consistent with the quantisation of the fluxes as was shown in [268, 269].

[5] However, in this approach it was not clear any more whether the hypersurface deformation algebra closes, which should

can be embedded in any way into σ, hence especially such that its dual presents a decomposition of the hypersurface. Then, the holonomies of $\hat{C}^\epsilon$ must be regularised in such a way that they keep the discretisation as it is, e.g. attach loops along the minimal plaquettes adjacent to a vertex v, see figure V.1.[6] If only finitely many edges of this graph are excited then we establish with this construction the correspondence to systems with finitely many degrees of freedom. Thus, we are now in a situation where the *quantisation ambiguities* of different regularisations can be studied via the same methods of cylindrical consistency we motivated in *III. Renormalisation*.

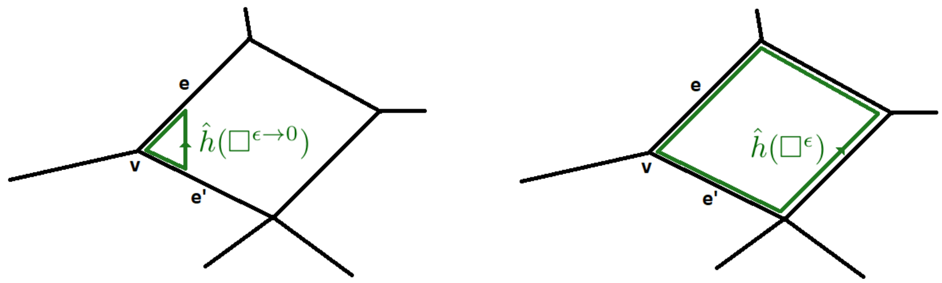

Abbildung V.1: Different ways to regularise the holonomy along a loop starting at v, as it appears in $\hat{C}^\epsilon$. On the left, the graph-changing regularisation is shown. On the right, the non graph-changing version, by which a single graph can be considered as a discretisation of σ is depicted. Here, the regularisation ambiguities can hopefully be treated via the direct Hamiltonian renormalisation.

Indeed, that different regularisations lead to severe changes of the physical predictions on some finite resolution can be seen in a concrete example: a semi-classical universe imitating a variant of the flat Robertson-Walker model. For this, we choose a cubic graph $\gamma := \cup_{I\in\mathcal{I}} e_I, \quad \mathcal{I} = \{(k,m) \ : k \in \mathbb{Z}^3_M, m \in \{1,2,3\}\}$ with $M < \infty$ and periodic boundary conditions. Then, we embed this graph into the manifold $\sigma = [0,1)^3$ such that the M^3 points are evenly distributed with respect to some fiducial metric[7]. In this coordinate metric the distance between two neighbouring points reads $\epsilon = 1/M$. Finally, we choose as the element of $\mathcal{H}_{kin}$ describing the system the vector $\Psi_{(c,p)} \in \mathcal{H}_\gamma$, which is a direct product of gauge coherent states peaked on edges in the (flat) Robertson-Walker metric.
This procedure is made precise in *V.C. Cosmological Coherent States Expectation Values*. Here, we will prepare the necessary tools in order to evaluate the expectation value of the scalar constraint in its non graph-changing regularisation on these *cosmological coherent states* $\Psi_{(c,p)}$. The calculation, as has been performed in [133], relies heavily on the fact that the expectation value on complexifier coherent states of operators with a polynomial dependence on the volume operator can be considerably simplified. In [94], it was shown that

$$\langle\Psi_{(c,p)} \ , \ P(\ \hat{V}_{AL}\ )\ \Psi_{(c,p)}\rangle \ = \ \langle\Psi_{(c,p)} \ , \ P(\ \hat{V}^k_{GT}\ )\ \Psi_{(c,p)}\rangle \ + \ \mathcal{O}(t^{k+1}) \tag{V.5}$$

for any polynomial P. Here, $\hat{V}^k_{GT}$ is the k-th *Giesel-Thiemann volume*, which is a mere power series in $\hat{Q}_v$. Hence, the original problem of finding the spectrum of $\hat{Q}_v$ can be circumvented as long as we are interested only in corrections up to a finite order $k+1$ in $t \sim \hbar$.
It is then an algebraic task to determine the expectation value of polynomials in holonomies and fluxes on each edge. We present their analytic form for arbitrary powers in the fluxes and up to quadratic order in the holonomies. To obtain the corresponding expression of a geometric operator, it is a combinatorial task to put these single building blocks together. We show the procedure in the case of the volume operator explicitly and we will, moreover, provide a general algorithm by which more complicated operators, such as the scalar constraint itself, can be investigated. It is of no surprise that we find in [132] that the expectation value of $\hat{C}^\epsilon$ coincides at the zeroth order in $\hbar$ with the classical discretisation C^ϵ as derived in (IV.239):

$$\langle\Psi_{(c,p)}, \hat{C}^\epsilon[1]\Psi_{(c,p)}\rangle \ = \ \frac{6V_0}{\kappa}\sqrt{p}\left(\frac{\sin(\epsilon c)^2}{\epsilon^2} - \frac{1+\beta^2}{\beta^2}\frac{\sin(2\epsilon c)^2}{4\epsilon^2}\right) \ + \ \mathcal{O}(\hbar), \tag{V.6}$$

be the case if the regularised operator were to describe a quantum theory of GR. To deal with this, one introduced the master constraint approach [86–91].

[6]This action is moreover diffeomorphism invariant, as under the action of $\varphi \in \text{Diff}(\sigma)$ it gets transformed together with the graph γ. In this sense one can call the graph "abstract" and only needs to deal with a subset of residual diffeomorphisms, i.e. those which map the graph into itself.

[7]While, the model for the flat $k=0$ Robertson-Walker metric is defined on $\sigma = \mathbb{R}^3$, we choose here a toy model, where we study the same metric on a compact torus.

where V_0 is the coordinate volume of σ. As we have already discussed earlier, there are even more classical discretisations. They can feature increasingly smaller errors in the regularisation parameter ϵ, however all of them predict different times for the Bounce. It transpires that the details of the *Big Bounce* which resolves the singularity via an *effective Hamiltonian* are not necessarily meaningful. In order to understand whether one should trust (V.6) or the dynamics of the effective Hamiltonian from some other model, it is mandatory to do more work and fix the quantisation ambiguities related with the dynamics.

We want to close this chapter with a remark that these ambiguities even appear in symmetry reduced models of QG, see *V.D. Loop Quantisation of Symmetry Reduced Models*. One might hope that due to the high degree of symmetries these models simplify enough such that these ambiguities do not occur anymore. However, at least in the considered model this is not the case.
The most promising candidate is *Loop Quantum Cosmology*, where prior to quantisation one classically restricts oneself to flat Robertson-Walker spacetime deparametrised by a dust field. Being an isotropic and homogeneous universe, the system loses its field-type behaviour: the only freedom left over is the scale factor $a(t)$. To stay as closely as possible to LQG, the variables chosen to quantise are the volume of a fiducial cell of the universe (or the compact manifold σ mentioned above) and its conjugate momentum. This has been done first in [80, 81]. Since then it has been of increasing success and was investigated further, e.g. in [82–85, 282, 283]. It became common to integrate further features from full Loop Quantum Gravity into this framework, most notably the aforementioned finite area gap Δ. Demanding that the area of any loop while regularising the Hamiltonian should not be smaller than Δ, introduced a compactification $\sin(\epsilon c)/\epsilon$ of c, the coordinate time derivative of the scale factor. Then one quantises, e.g., the scalar constraint analogously to full QG. However, due to the finite parameter Δ, which has been introduced, the system became susceptible to different choices in the regularisation of the Hamiltonian, too. On the other hand, this model featured a resolution of the Big Bang in form of a Big Bounce. Furthermore, it is simple enough to study numerically the exact evolution of a coherent state in the quantum cosmology Hilbert space through the mentioned Bounce. This has been done for the first time in [284–286] using a regularisation which is widely spread in the literature. However, by choosing the regularisation suggested in [288–290], which is taking the analogous regularisation steps leading to (V.6), one obtains a vastly different picture [134]. We will compare these two cases in detail in the following sections. Moreover, it is interesting to note that, although both systems are highly non-trivial, the evolution of the volume $v \sim a(t)^{3/2}$ given by the effective Hamiltonian defined as the expectation value on the coherent states follows in each case the trajectory of the mean value of the quantum state (a function over the volume v) perfectly, hence justifying the prescript "effective".
All in all, this shows that even in LQC the dynamics is not reliable unless the quantisation ambiguities have been fixed. However, thanks to the previous active research in this field, all the tools are available to closely investigate their influence. As a possible avenue to fix the ambiguities renormalisation group techniques can be pinpointed, one incarnation thereof - which is purely in a Hamiltonian setting - has been discussed during the course of this thesis.

V.A Kinematical Hilbert space of LQG

V.A.1 The unique $\mathrm{Diff}(\sigma)$-invariant Ashtekar-Isham-Lewandowski State

The starting point for the quantisation of the kinematical Hilbert space is the holonomy-flux algebra from Lemma IV.C.5. To construct it, we consider the connection $A_a(x)$ along any curve e in the manifold to construct the *holonomy* $h(e) \in \mathrm{SU}(2)$, i.e. the path-ordered exponential of the connection along e. Similarly, we smear the densitised triad E^a against any 2-dimensional surface S to obtain the *flux* $E(S) \in \mathfrak{su}(2)$. For a curve e and a surface S we thus had

$$h(e) := \mathcal{P}\exp\left(\int_0^1 dt A_a(e(t))\dot{e}^a(t)\right), \quad E^I(S) := \int_S \epsilon_{abc} dx^a \wedge dx^b E^c_J \delta^{IJ} \tag{V.7}$$

The set of (h, E) along *all* curves and surfaces constitutes the *holonomy-flux algebra*.
As in this algebra all curves and surfaces are contained, there are also especially those which are only continuous and not differentiable. To exclude them in the following, we follow the strategy of [50, 258] and consider only a subset of the holonomy-flux algebra, namely those elements which are defined with respect to *piecewise analytic* surfaces and curves:[8]

[8] We demand certain analytic structures to avoid, for example, situations where a curve and a surface would intersect in infinitely many points. On the other hand, we don't want to demand more, e.g. entire analyticity: diffeomorphisms preserving such a structure would be non-trivial everywhere, if they are non-trivial in an arbitrary small neighbourhood.

Definition V.A.1. *1) A curve is called* piecewise analytic *if it contains finitely many real analytic segments which meet in their boundaries. A real analytic segment is called an edge e.*
2) A piecewise analytic *surface is a finite union of real analytic surfaces called faces as follows:*

- *A face is an entire analytic 2-manifold without boundaries*
- *The faces are mutually disjoint and their closures meet in 1-dim submanifolds which themselves are piecewise analytic paths*
- *The closure of the surface is a C^0 2-dim connected submanifold contained in a compact set*
- *The surface is orientable*

One can use this to define the Hilbert space by GNS construction. We sketch the main idea in the following:

Definition V.A.2 (Cylindrical functions)**.** *1) A* graph *γ is a finite collection of edges $e \in \gamma$ (Alternatively we refer to the set of all edges in γ as $E(\gamma)$). The set of* vertices *of γ shall be denoted by $V(\gamma)$.*
2) A function F on the space of smooth connections is said to be cylindrical *over γ, i.e. $F \in \mathrm{Cyl}^\infty$,iff there exists $F_\gamma : \ \mathrm{SU}(2)^{|E(\gamma)|} \to \mathbb{C}$ such that*

$$F(A) = F_\gamma(\{h(e)\}_{e\in E(\gamma)}) = (p_\gamma^* F_\gamma)(A) \tag{V.8}$$

where $p_\gamma(A) = \{h(e)\}_{e\in E(\gamma)}$.
3) Let be $\lambda_h : \mathrm{SU}(2) \to \mathrm{SU}(2),\ g \mapsto hg$ the diffeomorphism of left translation. For $\tau = c_J \tau_J \in \mathfrak{su}(2)$ we define the generator of left translation in direction τ or right-invariant vector field

$$(R_\tau f)(g) = \frac{d}{ds}\,|_{s=0}\,(\lambda^*_{\exp(s\tau)} f)(g) \tag{V.9}$$

4) With every flux $E_f(S)$ (S being a surface and $f : \sigma \to \mathfrak{su}(2)$) we associate a derivative *$\hat{E}_{f,S}$ on the space of cylindrical functions:*

$$\hat{E}_{f,S} F := \{E_f(S), F\} = \frac{\beta\kappa}{2} \sum_e \sigma(S,e) R_{f(S\cap e)}(e) F_\gamma \tag{V.10}$$

where $R(e)$ acts only on the e-th copy of $\mathrm{SU}(2)$ in F_γ.

These objects will now give rise to the quantum algebra $\hat{\mathcal{A}}$ in LQG: namely consider $\tilde{\mathcal{E}}$ the set of all pairs $(\hat{E}, F)$ with F being a cylindrical function $F \in \mathrm{Cyl}^\infty$ (such that there exists for each function a graph γ with finitely many edges) and $\hat{E}$ being only one of those derivations which are of the form $\hat{E}_{f,S}$ with S being a piecewise analytic surface. For two elements $l = (\hat{E}, F),\ l' = (\hat{E}', F')$ we define the involution $l^* = (\hat{E}^*, F^*)$ as the complex conjugation of the entries and the Lie bracket as

$$[l, l'] = \Big([\hat{E}, \hat{E}'], \hat{E}(F') - \hat{E}'(F)\Big) \tag{V.11}$$

To obtain the subset mentioned in Def II.B.1 with whom the GNS construction can be undergone, we will call $\mathcal{E}$ the set of all elements generated from $\tilde{\mathcal{E}}$ by (V.11). Hence, the set is by construction such that we can construct the free algebra along the lines of (II.73)-(II.75) out of it. This finishes the formal construction of the quantum algebra $\hat{\mathcal{A}}$.

To talk about the action of diffeomorphisms on $\hat{\mathcal{A}}$, we generalise the class of diffeomorphisms to allow also those, which act non-trivial only in a compact set. Hence, these diffeomorphisms will not be analytic everywhere, but only differentiable (to some order) at the boundary of the chosen compact set. These diffeomorphisms motivated us to consider only piecewise analytic edges and surfaces. Then, the diffeomorphisms will preserve the structure of the edges and surface, i.e. they are automorphisms on $\hat{\mathcal{A}}$. (see [258] for more details)
It turns out that for the holonomy-flux $\star$-algebra there is only one state which is invariant with respect to all of these diffeomorphisms:

Theorem V.A.1. *(Lewandowski, Okolow, Sahlmann, Thiemann, '06 & Fleischhack '09) The only diffeomorphism invariant state on the quantum holonomy-flux algebra $\hat{\mathcal{A}}$ is the so-called Ashtekar-Isham-Lewandowski state*

$$\omega_{AL}(F(A)\ \star \hat{E}_{f_1}(S_1)...\hat{E}_{f_N}(S_N)) = \begin{cases} 0 & \text{if} N > 0 \\ \mu_H(F) & \text{else} \end{cases} \tag{V.12}$$

where

$$\mu_H(F) = \int_{\mathrm{SU}(2)^{|E(\gamma)|}} \prod_{e\in E(\gamma)} d\mu_H(g_e) F_\gamma(\{g_e\}) \tag{V.13}$$

with $F = p_\gamma^* F_\gamma$ *is cylindrical over* γ.

Beweis. For the proof we refer to the literature. A didactic presentation can be found in [50]. □

V.A.2 GNS Construction and the kinematical Hilbert Space $\mathcal{H}_{kin}$

We will now state the result of the GNS construction of ω_{AL} on a fixed graph $\gamma = \cup_I e_I$. The associated Hilbert space to γ is the tensor product of square integrable functions on each edge, $\mathcal{H}_\gamma = \otimes_{e\in E(\gamma)}\mathcal{H}_e$ with $\mathcal{H}_e = L_2(\mathrm{SU}(2), d\mu_H)$, $d\mu_H$ being the unique Haar measure on SU(2). The holonomies get promoted to bounded, unitary multiplication operators: for $f_e \in \mathcal{H}_e$ it is

$$\hat{h}_{mn}(e)f_e(g) := D^{(\frac{1}{2})}_{mn}(g)f_e(g) \tag{V.14}$$

where $D^{(\frac{1}{2})}_{mn}(g)$ is the Wigner-matrix of group element g in the defining irreducible representation of SU(2) corresponding to spin-1/2 [291]. The Peter-Weyl Theorem II.A.5 ensures that the functions $D^{(j)}_{mn}(g)$ form an orthogonal basis, hence $\mathcal{H}_e$ is the closure of functions of the form $f_e(g_e) = \sum_j \sum_{-j\le m,n\le j} c_{jmn} D^{(j)}_{mn}(g_e)$, where $j \in \mathbb{N}/2$ (sums over magnetic indices $m, n, ...$ will be suppressed in the following). Now, as $\mathcal{H}_\gamma = \otimes_{e\in E(\gamma)}\mathcal{H}_e$, an orthogonal basis of it are the *spin-network functions* [274–276]

$$T_{\gamma,\vec{j},\vec{m},\vec{n}}(\{g\}) := \prod_{e\in E(\gamma)} D^{(j_e)}_{m_e n_e}(g_e) \tag{V.15}$$

The scalar product between two spin-network functions $T_{\gamma,\vec{j},\vec{m},\vec{n}}, T_{\gamma',\vec{j}',\vec{m}',\vec{n}'}$, which are defined on two different graphs γ, γ', is defined in the following way: Choose any $\tilde{\gamma}$ such that $\gamma \subseteq \tilde{\gamma}$ and $\gamma' \subseteq \tilde{\gamma}$. Then we define

$$T_{\tilde{\gamma},\vec{j}^\sim,\vec{m}^\sim,\vec{n}^\sim} := \prod_{e\in E(\gamma)} D^{(j_e)}_{m_e n_e}(g_e) \prod_{e\in\tilde{\gamma}-\gamma} D^{(0)}_{00}(g_e) \tag{V.16}$$

and similar we extend $T_{\gamma',\vec{j}',\vec{m}',\vec{n}'}$ to $\tilde{\gamma}$. Now, both functions are defined on the same graph and their scalar product can be compute in the L_2 sense: (we rename $\vec{j} := \vec{j}^\sim$ and similar)

$$\langle T_{\tilde{\gamma},\vec{j},\vec{m},\vec{n}}, T_{\tilde{\gamma},\vec{j}',\vec{m}',\vec{n}'}\rangle = \prod_{e\in\tilde{\gamma}} \int d\mu_H(g_e) \overline{D^{(j_e)}_{m_e n e}(g_e)} D^{(j'_e)}_{m'_e n'_e}(g_e) \tag{V.17}$$

$$\int d\mu_H(g) \overline{D^{(j)}_{mn}(g)} D^{(j')}_{m'n'}(g) = \frac{1}{d_j}\delta_{jj'}\delta_{mm'}\delta_{nn'} \tag{V.18}$$

where the dimension of spin-j SU(2)-irrep is $d_j = 2j+1$. Similarly, the fluxes become essentially self-adjoint derivation operators:

$$\hat{E}^K(S)f_e(g) := -\frac{i\hbar\kappa\beta}{2}\sigma(e\cap S)f_{e_1}(g_{e_1})R^K(e_2)f_{e_2}(g_{e_2}) \tag{V.19}$$

where $\sigma(e\cap S) \in \{0, \pm 1\}$ (depending on whether edge and surface meet non-transversally or under the same/opposite orientation respectively), $e = e_1 \circ e_2$ such that $s_e = e\cap S$ is the starting point of edge e_2 and $g = g_{e_1}g_{e_2}$ (which makes the splitting unique). Finally, the *right-invariant vector field* $R^K(e)$ was defined in (V.9) and in the same way the *left-invariant vector field* $L^K(e)$ is defined as

$$R^K(e)f_e(g) := \frac{d}{ds}\Big|_{s=0} f_e(e^{s\tau_K}g), \qquad L^K(e)f_e(g) := \frac{d}{ds}\Big|_{s=0} f_e(ge^{s\tau_K}) \tag{V.20}$$

Let us note, that in general we need indeed all graphs consisting of piecewise analytic edges, because the algebra of observables contains the holonomies along all these paths. And, if some paths were missing, these could be obtained through the natural action of some element of the diffeomorphism group (see later).
However, there are also different ways to implement the action of the diffeomorphism group, e.g., in Algebraic

Quantum Gravity [92] one considers an abstract (or algebraic) graph that is not embedded and only carries the information which vertices are connected with each other. One can quantise the action of the infinitesimal diffeomorphisms[9] such that they preserve the algebraic graph and, hence, it suffices indeed to take only one abstract graph into account.

As we are in the following interested in a non graph-changing regularisation of our observables, we will also consider a single graph γ that defines a complete set of coordinates of the phase space which are to become elementary operators. Moreover, let γ be such that we can define a polyhedral decomposition of σ dual to γ in the following way designed by [154]: to each edge e of γ we assign an open face S_e carrying the same orientation as e and such that (1) the faces S_e are mutually non-intersecting, (2) only e intersects S_e and (3) the intersection happens only in one point infinitesimal close the starting point of e and is transversal.
Then (V.19), the action of $\hat{E}^K(S_e)$ on a cylindrical function of γ, becomes proportional to the action of the right-invariant vector field $R^K(e)$. However, note that the fluxes now longer commute with each other. In other words, we find the resulting algebra on the mentioned given graph γ with edges e, e':

$$[\hat{h}_{ab}(e), \hat{h}_{cd}(e')] = 0, \qquad [R^K(e), R^L(e')] = \delta_{ee'}\epsilon^{KL}{}_M R^M(e)$$
$$[R^K(e), \hat{h}_{ab}(e')] = \delta_{ee'} D'^{(\frac{1}{2})}_{ac}(\tau_K)\hat{h}_{cb}(e) \tag{V.21}$$

with $D'^{(\frac{1}{2})}_{ab}(\tau_K)$ as defined in (V.23). This is taken from [133], where it was explicitly computed in the *spherical basis*, $s \in \{-1, 0, +1\}$, where $\tau_\pm := \mp(\tau_1 \pm i\tau_2)/\sqrt{2}$ and $\tau_0 := \tau_3$. The generators thereof are

$$\tau_+ = i\sqrt{2}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \tau_- = -i\sqrt{2}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \tau_0 = -i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{V.22}$$

Lemma V.A.1. *Let $K \in \{0, \pm 1\}$, then the action of R^K on the basis element is given by*

$$R^K D^{(j)}_{mn}(g) := D'^{(j)}_{m\mu}(\tau_K) D^{(j)}_{\mu n}(g), \quad D'^{(j)}_{mn}(\tau_K) = 2i\sqrt{j(j+1)d_j}(-1)^{j+n}\begin{pmatrix} j & 1 & j \\ n & K & -m \end{pmatrix} \tag{V.23}$$

Beweis. First, recall that $R^K f(g) = (d/ds)_{s=0} f(e^{s\tau_K} g)$, so replacing f with $D^{(j)}_{mn}$, we get

$$R^K D^{(j)}_{mn}(g) = \left(\frac{d}{ds}\right)_{s=0} D^{(j)}_{mn}(e^{s\tau_K} g) = \sum_\mu \left(\frac{d}{ds}\right)_{s=0} D^{(j)}_{m\mu}(e^{s\tau_K}) D^{(j)}_{\mu n}(g) \tag{V.24}$$

so comparison with the definition in (V.23) reveals that

$$D'^{(j)}_{m\mu}(\tau_K) = \left(\frac{d}{ds}\right)_{s=0} D^{(j)}_{m\mu}(e^{s\tau_K}) \tag{V.25}$$

so we are left with the task of performing this derivative. Given $\tau_\pm$ and τ_0, it is easy to see that $e^{s\tau_K} = \sum_{n=0}^\infty s^n(\tau_K)^n/n!$ gives

$$e^{s\tau_+} = \begin{pmatrix} 1 & is\sqrt{2} \\ 0 & 1 \end{pmatrix}, \qquad e^{s\tau_-} = \begin{pmatrix} 1 & 0 \\ -is\sqrt{2} & 1 \end{pmatrix}, \qquad e^{s\tau_0} = \begin{pmatrix} e^{-is} & 0 \\ 0 & e^{is} \end{pmatrix} \tag{V.26}$$

Consider for instance τ_+. From [50] we have

$$D'^{(j)}_{mn}(\tau_+) = \sum_l \frac{\sqrt{(j+m)!(j-m)!(j+n)!(j-n)!}}{(j+n-l)!(m-n+l)!l!(j-m-l)!} \left.\frac{d}{ds}\right|_{s=0} b^{m-n+l} c^l \tag{V.27}$$

with $b = is\sqrt{2}$ – so that the derivative in s gives $i\sqrt{2}(m-n+l)b^{m-n+l-1}$ – and $c = 0$. The only way for this not to vanish is to have $l = 0$ (so that the sum collapses in a single term) and $m - n - 1 = 0$, i.e. $\delta_{m,n+1}$. For these values the factorials simplify, and the final formula is

$$D'^{(j)}_{mn}(\tau_+) = i\sqrt{2}\sqrt{(j+n+1)(j-n)}\delta_{m,n+1} \tag{V.28}$$

[9] To be precise, one is not quantising $\vec{C}$ there, but a classically equivalent term which is part of the Master constraint.

Similar computations reveal that

$$D'^{(j)}_{mn}(\tau_-) = -i\sqrt{2}\sqrt{(j-n+1)(j+n)}\delta_{m,n-1} \tag{V.29}$$

and

$$D'^{(j)}_{mn}(\tau_0) = -2in\delta_{mn} \tag{V.30}$$

It is convenient to write these in terms of $3j$-symbols, as in this way we have a unique formula and the symmetry properties of these objects are apparent. Recalling the explicit formulae for $3j$-symbols [291]

$$\begin{aligned} \begin{pmatrix} j & 1 & j \\ n & 0 & -m \end{pmatrix} &= \delta_{mn}(-1)^{j+n+1}\frac{n}{\sqrt{j(j+1)d_j}} \\ \begin{pmatrix} j & 1 & j \\ n & \pm 1 & -m \end{pmatrix} &= \pm\delta_{m,n\pm 1}(-1)^{j+n}\sqrt{\frac{(j\mp n)(j\pm n+1)}{2j(j+1)d_j}} \end{aligned} \tag{V.31}$$

one can therefore write

$$D'^{(j)}_{mn}(\tau_K) = 2i\sqrt{j(j+1)d_j}(-1)^{j+n}\begin{pmatrix} j & 1 & j \\ n & K & -m \end{pmatrix} \tag{V.32}$$

which is the claim. □

This concludes the description on the *kinematical Hilbert space* of LQG.

V.A.3 (Gauge) Complexifier Coherent States

We now have at our disposal a physical Hilbert space on the fixed graph γ. But while any state $F \in \mathcal{H}_\gamma$ can be considered, later on we will focus on a subset of the *gauge coherent state* family. Let us therefore briefly review the general definition and properties of this family as it was introduced in [154–156].

Following Hall [263, 264], one constructs a coherent state $\psi^t_{e,h^{\mathbb{C}}_e}$ for every edge e of the graph and forms the tensor product over all edges. Explicitly, we obtain $\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}(\{g\}) := \prod_{e\in E(\gamma)}\psi^t_{e,h^{\mathbb{C}}_e}(g_e)$. To construct $\psi^t_{e,h^{\mathbb{C}}_e}$ one uses a complex polarisation of the classical phase space, i.e. a unitary map $(A,E)\mapsto A^{\mathbb{C}}$ that expresses the complex connection as a function of the real phase space. For example, the left-polar decomposition prescribes

$$h^{\mathbb{C}}_e := \exp\left(-\frac{it}{\hbar\kappa\beta}\tau_J E^J(S_e)\right) h(e) \in SL(2,\mathbb{C}) \tag{V.33}$$

where $h(e)$ is the classical holonomy along edge e and $E^J(S_e)$ are defined with respect to the surfaces S_e for each edge e as described above. The dimensionless quantity $t := \hbar\kappa/\ell^2 > 0$ is called the *semiclassicality parameter*, with ℓ being a length scale that the theory should provide.[10]

To construct the coherent state in $\mathcal{H}_e$ peaked on $h^{\mathbb{C}}_e \in SL(2,\mathbb{C})$, one first chooses a *complexifier* $\hat{C}_{t,e}$ and exponentiates it: this gives rise to the coherent state transform, which for the choice of heat kernel complexifier [154] reads

$$\hat{W}_{t,e} := e^{-\frac{1}{\hbar}\hat{C}_{t,e}} = e^{\frac{t}{8}\delta_{IJ}R^I(e)R^J(e)} \tag{V.34}$$

The *(gauge-variant) coherent state* is now obtained by applying $\hat{W}_{t,e}$ to the delta-function on SU(2), $\delta_{h'}$, and continuing analytically the result to $h' \to h^{\mathbb{C}}_e$:

$$\psi^t_{e,h^{\mathbb{C}}_e}(g) := \left(\hat{W}_{t,e}\delta_{h'}(g)\right)_{h'\to h^{\mathbb{C}}_e} = \sum_j d_j e^{-\frac{t}{2}j(j+1)}\mathrm{Tr}^{(j)}((h^{\mathbb{C}}_e)^\dagger g) \tag{V.35}$$

where $\mathrm{Tr}^{(j)}(.)$ denotes the trace in the spin-j irreducible representation and the explicit expression $\delta_h(g) = \sum_j d_j \mathrm{Tr}^{(j)}(hg^{-1})$ has been used.

As was shown in [155], these coherent states fulfil a number of useful properties:

[10] As we will see later, t controls the spread in holonomy and flux of the coherent state: The smaller t, the smaller the relative dispersions of h and E. It has been therefore argued [94] that the natural choice for ℓ^2 in a vacuum gravity context is the inverse of cosmological constant, $\ell^2 = 1/\Lambda$. Using $\kappa = 16\pi G/c^3$, one then finds $t \sim 10^{-120}$.

(1) *Eigenstates of an annihilation operator.* By defining $\hat{a}(e) := e^{-\frac{1}{\hbar}\hat{C}_{t,e}}\hat{h}(e)e^{\frac{1}{\hbar}\hat{C}_{t,e}} = e^{\frac{3t}{8}}e^{-i\tau_I\hat{E}^I(S_e)/2}\hat{h}(e)$ (where the action of the last exponential has to be understood via Nelson's analytic vector theorem, see e.g. page 202 of [186]), one finds that the coherent states are simultaneous eigenstates for each $\hat{a}(e)$:

$$\hat{a}_{mn}(e)\Psi^t_{\gamma,\{h^{\mathbb{C}}\}} = [h^{\mathbb{C}}_e]_{mn}\Psi^t_{\gamma,\{h^{\mathbb{C}}\}} \tag{V.36}$$

(2) *Overcompleteness relation.* By considering the measure ($p_J \in \mathbb{R}, h_e \in \mathrm{SU}(2)$)

$$d\nu_t(e^{i\tau_J p_J/2}h_e) := d\mu_H(h_e)[\frac{2\sqrt{2}e^{-t/4}}{(2\pi t)^{3/2}}\frac{\sinh(\sqrt{p^2})}{\sqrt{p^2}}e^{-p^2/t}dp^3] \tag{V.37}$$

on $\mathrm{SL}(2,\mathbb{C})$, one can show that

$$\int_{\mathrm{SL}(2,\mathbb{C})} d\nu_t(h^{\mathbb{C}}_e)\ \psi^t_{e,h^{\mathbb{C}}_e}\ \langle\psi^t_{e,h^{\mathbb{C}}_e},\cdot\rangle = \mathbb{1}_{\mathcal{H}_e} \tag{V.38}$$

(3) *Sharp peakedness in holonomy and electric flux.* For all $h, h' \in \mathrm{SL}(2,\mathbb{C})$ there exists a positive function $K_t(h,h')$ decaying exponentially fast as $t \to 0$ for $h \neq h'$ and such that

$$|\ \langle\psi^t_h,\psi^t_{h'}\rangle\ |^2 \leq K_t(h,h')||\psi^t_h||^2||\psi^t_{h'}||^2 \tag{V.39}$$

Moreover, for holonomies and fluxes one finds

$$\langle\psi^t_h,\hat{h}_{mn}(e)\psi^t_{h'}\rangle = h_{mn}(e)\langle\psi^t_h,\psi^t_{h'}\rangle + \mathcal{O}(t) \tag{V.40}$$

$$\langle\psi^t_h,\hat{E}^J(S_e)\psi^t_{h'}\rangle = E^J(S_e)\langle\psi^t_h,\psi^t_{h'}\rangle + \mathcal{O}(t) \tag{V.41}$$

and that they saturate the Heisenberg uncertainty bound by occupying a phase space volume (with respect to the Liouville measure) of order t^3.

V.B Quantisation of Geometric Operators and Constraints

V.B.1 The Volume Operator

For the volume over a classical region $B \subset \sigma$ the process of canonical quantisation on a given graph γ uses the following regularisation:
We consider a partition of B into cubes $\square$ and get the classical identity

$$V(B) = \sum_\square \int_\square d^3u\ \sqrt{\det(X^*_B q)} \tag{V.42}$$

for an embedding function X_B into σ. We introduce the "face normals" of $\square$ at fixed values of u^b. Then we calculate

$$\det([E^a_J(X_B(u))n^b_a]^b_J) = \det(E^a_J)\cdot\det(n^b_a) = \det(E)(\det(\frac{\partial X_B}{\partial u}))^2 \tag{V.43}$$

and with

$$\det(X^*_B q) = (\det(\frac{\partial X_B}{\partial u}))^2\det(q) \tag{V.44}$$

we arrive at

$$\sqrt{\det(X^*Bq)} = \sqrt{|\det(E\cdot n)\ |} \tag{V.45}$$

Suppose that each $\square$ has coordinate volume ϵ^3 then ($u_\square \in \square$)

$$\int_\square d^3u\ \sqrt{\det(X^*_B q)} = \epsilon^3\sqrt{\det(X^*_B q)}(X^*_B(u_\square)) = \sqrt{|\det(E\cdot n\epsilon^2)|} \approx \sqrt{|\det(\{E_J(\square^b)\}^b_J)|} \tag{V.46}$$

where $E_J(\Box^b)$ is the flux through the b-th face of $\Box$. In the following we write in an abuse of notation $\det(E(\Box)) := \det(\{E_J(\Box)^b)\}^b_J)$. Thus, we finally obtain:

$$V(B) \approx \sum_{\Box} |\det(E(\Box))|^{1/2} + \mathcal{O}(\epsilon) \tag{V.47}$$

$$\det(E(\Box)) = \frac{1}{3!}\epsilon_{abc}\epsilon^{IJK}E_I(\Box^a)E_J(\Box^b)E_K(\Box^c) \tag{V.48}$$

We define this by its action on a spin-network function

$$\det(\hat{E}(\Box))T_{\gamma,\vec{j},\vec{m},\vec{n}} = \left(\frac{\hbar\kappa\beta}{2}\right)^3 \frac{1}{6}\times \tag{V.49}$$
$$\times \sum_{e,e',e'\in E(\gamma)} (\epsilon^{abc}\sigma(\Box^a,e)\sigma(\Box^b,e')\sigma(\Box^c,e''))\epsilon_{JKL}R^J(e)R^K(e')R^L(e''))T_{\gamma,\vec{j},\vec{m},\vec{n}}$$

As $\epsilon \to 0$ the only contributions comes from cubes that contain at least a trivalent vertex. Also, we can choose each cube to contain only one vertex at most, else we shrink ϵ further. This leads, finally, to the Ashtekar-Lewandowski volume operator [11] [266]

$$\hat{V}(B)F_\gamma(\{g\}) = \sum_{v\in V(\gamma)\cap B}\hat{V}_v F_\gamma(\{g\}) = \frac{(\beta\hbar\kappa)^{3/2}}{2^5\sqrt{3}}\sum_{v\in V(\gamma)\cap B}\sqrt{|\hat{Q}_v|}F_\gamma(\{g\}), \tag{V.50}$$

$$\hat{Q}_v := i\sum_{e\cap e'\cap e''=v}\epsilon(e,e',e'')\epsilon_{IJK}R^I(e)R^J(e')R^K(e'') \tag{V.51}$$

with $\epsilon(e,e',e'') := sgn(\det(\dot{e},\dot{e}',\dot{e}''))$ and all edges outgoing at the vertex v. (In case of an e being ingoing, one simply replaces $R^K(e) \to L^K(e)$.) Since the square-root is understood in the sense of the spectral theorem, knowledge of the full spectrum of $\hat{Q}_v$ is required before we can say how $\hat{V}_v$ acts on general states.

Important for the purposes we have in mind, is the advantage of using the coherent states to simplify the evaluation of expectation values of operators involving the Ashtekar-Lewandowski volume (V.50). Indeed, given a coherent state (which is peaked at each edge on $|h_{mn}(e)| \gg t$, $|E^J(S_e)| \gg t$), it was shown in [94] that for every polynomial operator $P(\hat{V}_v,\hat{h})$ the following relation holds:

$$\langle\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}, P(\hat{V}_v,\hat{h})\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}\rangle = \langle\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}, P(\hat{V}^{GT}_{k,v},\hat{h})\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}\rangle + \mathcal{O}(t^{k+1}) \tag{V.52}$$

where we refer to $\hat{V}^{GT}_v$ as the k-*th Giesel-Thiemann volume operator*. This is explicitly given by

$$\hat{V}^{GT}_{k,v} := \frac{(\beta\hbar\kappa)^{\frac{3}{2}}}{2^5\sqrt{3}}\sqrt{\langle\hat{Q}_v\rangle}\left[\mathbb{1}_{\mathcal{H}_\gamma} + \sum_{n=1}^{2k+1}\frac{(-1)^n}{n!}\left(0-\frac{1}{4}\right)\left(1-\frac{1}{4}\right)\dots\left(n-1-\frac{1}{4}\right)\left(\frac{\hat{Q}_v^2}{\langle\hat{Q}_v\rangle^2}-\mathbb{1}_{\mathcal{H}_\gamma}\right)^n\right] \tag{V.53}$$

where $\hat{Q}_v$ is as in (V.51) and we used the shorthand notation $\langle\hat{Q}_v\rangle := \langle\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}, \hat{Q}_v\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}\rangle$.[12] This fact enables us to compute the approximated expectation value (on these coherent states) of any polynomial operator involving Ashtekar-Lewandowski volume, retaining control on the error we make in terms of powers of the semiclassicality parameter t.

V.B.2 Gauss and Diffeomorphism Constraint

It remains to incorporate the constraints $G_J, \vec{C}[\vec{N}], C[N]$. The Gauss constraint G_J is easily incorporated by the fact that it is the generator of SU(2)-rotations, hence its solutions are states of $\mathcal{H}_\gamma$ which are invariant under SU(2). These can be obtained by group averaging: let $U_G[g]$ be the operator that generates a local $g(x) \in$ SU(2) transformation and $F_\gamma(\{g\}) = \prod_{e\in\gamma} f_e(g_e)$, i.e. a tensor product over the edges; then the corresponding gauge-invariant function is [292, 293]

$$F^G_\gamma(g) = \int D[\{h\}]U_G[\{h\}]F_\gamma(\{g\}) := \left(\prod_{v\in V(\gamma)}\int d\mu_H(h_v)\right)\prod_{e\in\gamma} f_e(h_{s_e} g h^{-1}_{t_e}) \tag{V.54}$$

[11] We can take care of the non-commutative nature of the $\hat{E}$ by introducing a regularisation procedure called "link-splitting" [50]. With this one can show that all contributions where $\hat{E}$ acts on its copy of a different surface cancel.

[12] We observe that the operator $\hat{V}^{GT}_{k,v}$ depends explicitly on the coherent state $\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}$ which appears in (V.52), and it therefore makes sense only in the context of equation (V.52).

where v runs through all vertices in γ, and s_e, t_e denote the vertex at the beginning/end of edge e respectively. Assume one implements the Gauss constraint via group averaging and is only interested in the expectation value of observables which are themselves gauge-invariant (like we have already established for the scalar constraint). These are $\hat{O}_F$ such that $U_G[g]^\dagger \hat{O}_F U_G[g] = \hat{O}_F$ for any SU(2) transformation $U_G[g]$. Moreover, it is easy to see by (V.35) that the coherent states are *gauge-covariant*: for a gauge transformation of $\tilde{g}$ at $x = s_e$, the starting point of edge e, we get $U_G[\tilde{g}]\psi^t_{e,h^{\mathbb{C}}_e}(g) = \psi^t_{e,h^{\mathbb{C}}_e}(g\tilde{g}) = \psi^t_{e,h^{\mathbb{C}}_e\tilde{g}^\dagger}(g)$. Conversely, for $x = t_{e'}$ the terminal point of edge e', it is $U_G[\tilde{g}]\psi^t_{e',h^{\mathbb{C}}_{e'}}(g) = \psi^t_{e',h^{\mathbb{C}}_{e'}}(\tilde{g}g) = \psi^t_{e',\tilde{g}^\dagger h^{\mathbb{C}}_{e'}}(g)$. Combining both with the fact that the coherent states are sharply peaked, we get

$$
\begin{aligned}
\langle \Psi^G_{(c,p)}, \hat{O}_F \Psi^G_{(c,p)}\rangle &= \int D[\{\tilde{g}\}] \int D[\{\tilde{g}'\}] \prod_{e\in E(\gamma)} \langle \psi_{e,H_e}, U_G[\tilde{g}_{s_e}]^\dagger U_G[\tilde{g}_{t_e}]^\dagger \hat{O}_F U_G[\tilde{g}'_{s_e}] U_G[\tilde{g}'_{t_e}] \psi_{e,H_e}\rangle \\
&= \int D[\{\tilde{g}\}] \int D[\{\tilde{g}'\}] \prod_{e\in E(\gamma)} \langle \psi_{e,\tilde{g}^{-1}_{t_e} H_e \tilde{g}^{-1}_{s_e}}, \hat{O}_F \psi_{e,\tilde{g}'^{-1}_{t_e} H_e \tilde{g}'^{-1}_{s_e}}\rangle \\
&= \int D[\{\tilde{g}\}] \int D[\{\tilde{g}'\}] \prod_{e\in E(\gamma)} \langle \psi_{e,\tilde{g}^{-1}_{t_e} H_e \tilde{g}^{-1}_{s_e}}, \hat{O}_F \psi_{e,\tilde{g}^{-1}_{t_e} H_e \tilde{g}^{-1}_{s_e}}\rangle \delta(\tilde{g},\tilde{g}') + \mathcal{O}(t) \\
&= \int D[\{\tilde{g}\}] \langle \Psi_{(c,p)}, U_G[\tilde{g}]^\dagger \hat{O}_F U_G[\tilde{g}] \Psi_{(c,p)}\rangle + \mathcal{O}(t) \\
&= \langle \Psi_{(c,p)}, \hat{O}_F \Psi_{(c,p)}\rangle + \mathcal{O}(t)
\end{aligned}
\tag{V.55}
$$

where in the second-to-last step we used the peakedness property of coherent states to write $\langle \psi_{e,H_e}, \hat{O}_F \psi_{e,H'_e}\rangle = \langle \psi_{e,H_e}, \hat{O}_F \psi_{e,H_e}\rangle \delta(H_e, H'_e) + \mathcal{O}(t)$, while in the last step we used the fact that the Haar measure is normalised. We see also that the normalisation of the state obeys $||\Psi^G_{(c,p)}|| = ||\Psi_{(c,p)}|| + \mathcal{O}(t)$. This result guarantees that the expectation values have physical significance at leading order in t (i.e. $\mathcal{O}(t^0)$), without having to impose the Gauss constraint. In other words, the expectation value of gauge invariant observables does at classical order not dependent on the representative of the gauge orbit of the phase space point. Of course, the corrections could be very large, thus the parameter t should be considered sufficiently small $t \to 0$. Further results on the general gauge-invariant coherent states can be found in [294, 295].

The vector constraint $\vec{C}[\vec{N}]$ generates diffeomorphisms of the spatial manifold σ, and therefore cannot be implemented as an infinitesimal operator due to the action of the diffeomorphism group Diff(σ) not being strongly continuous. Nevertheless, diffeomorphism-invariance can still be implemented via finite diffeomorphisms $\varphi \in$ Diff(σ). In this thesis, we adopt the idea developed in the context of AQG [92], where one considers *abstract graphs*, that is graphs which "forget" about their embedding in σ. In order to still reduce the number of degrees of freedom accordingly for our theory, we will introduce a classically equivalent constraint which can be promoted to an operator and implement it, instead of the vector constraint.
The object that is closely related to it – and that does admit a quantum counterpart – is $M := q^{ab} C_a C_b / \det(q)$ [50]. Let $\hat{M} = M(\hat{h}, \hat{E})$ be the corresponding operator, and let $\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}$ be a generic gauge coherent state. Then follows, from the peakedness property of coherent states [156],

$$
\langle \Psi^t_{\gamma,\{h^{\mathbb{C}}\}}, \hat{M}\Psi_{(c,p)}\rangle = M(h_o, E_o) \langle \Psi^t_{\gamma,\{h^{\mathbb{C}}\}}, \Psi_{(c,p)}\rangle + \mathcal{O}(t) \tag{V.56}
$$

where h_o and E_o represent schematically the leading orders (in t) of the expectation values of generic holonomy and flux on the cosmological coherent state $\Psi_{(c,p)}$. As we will see later, the leading order of these operators reproduces the classical value computed from data (c,p), so in fact we have $M(h_o, E_o) = M_{class}$. But now, we observe that the classical Robertson-Walker metric solves the spatial constraints identically (it is homogeneous, hence spatial derivatives vanish): $(C_a)_{class} = 0$. Since M is homogeneous in C_a, it immediately follows that $M_{class} = 0$, and so $\langle \Psi^t_{\gamma,\{h^{\mathbb{C}}\}}, \hat{M}\Psi_{(c,p)}\rangle$ vanishes at leading order in t. Since this is true for every $\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}$, and since the whole set of gauge coherent states forms a basis, we conclude that $\hat{M}\Psi_{(c,p)} = 0 + \mathcal{O}(t)$.
In this sense, even though the state $\Psi_{(c,p)}$ is not diff-invariant, expectation values computed with it have physical significance at leading order in t.

V.B.3 Quantisation of the Scalar Constraint

Finally, let us consider the implementation of the scalar constraint in the quantum theory. We had already introduced in the last chapter the regularisation due to Thiemann and, indeed, it could be used to implement for the first time a rigorous quantisation of the scalar constraint in LQG (we refer to [74, 75] for the details of this construction).

Non Graph-Changing Regularisation

Among the various choices of further regularisations proposed for the scalar constraint, we will use the framework first developed in AQG [93], where one chooses the scalar constraint to act in a *non graph-changing* way, i.e. one regularises the curvature of the Ashtekar connection by $F_{ab}(x)\dot{e}^a\dot{e}^b = [h(\Box_{ee'}) - h(\Box_{ee'})^\dagger]/2\epsilon^2 + \mathcal{O}(\epsilon)$ where $\Box_{ee'}$ denotes a small loop starting at x along e and returning along e' of coordinate length 4ϵ. Then, we choose for the action of the loop-holonomy the operator $\hat{h}(\Box_{ee'})$, which starts at a vertex v of the fixed graph γ and goes along already existing edges in such a way that minimally many edges are traversed. Thus, we simply define the total operator in its symmetrised version as follows:

$$\hat{C}[N] = \frac{1}{2}\left(\hat{C}_E[N] + \hat{C}_E^\dagger[N]\right) - \frac{\beta^2+1}{2\beta^2}\left(\hat{C}_L[N] + \hat{C}_L^\dagger[N]\right) \tag{V.57}$$

where the *Euclidian part* $\hat{C}_E$ and the *Lorentzian part* $\hat{C}_L$ are

$$\begin{aligned}\hat{C}_E[N] :=& \frac{32}{3i\kappa^2\hbar\beta}\sum_{v\in V(\gamma)}\frac{N_v}{20}\sum_{e\cap e'\cap e''=v}\epsilon(e,e',e'')\frac{1}{2}\times\\ &\times \mathrm{Tr}\left((\hat{h}(\Box_{ee'}) - \hat{h}(\Box_{ee'})^\dagger)\hat{h}(e'')\left[\hat{h}(e'')^\dagger, \hat{V}_v\right]\right) \qquad \text{(V.58)}\\ \hat{C}_L[N] :=& \frac{128}{3i\kappa^4\hbar^5\beta^5}\sum_{v\in V(\gamma)}\frac{N_v}{20}\sum_{e\cap e'\cap e''=v}\epsilon(e,e',e'')\times\\ &\times \mathrm{Tr}\left(\hat{h}(e)\left[\hat{h}(e)^\dagger, [\hat{C}_E[1], \hat{V}_v]\right]\hat{h}(e')\left[\hat{h}(e')^\dagger, [\hat{C}_E[1], \hat{V}_v]\right]\hat{h}(e'')\left[\hat{h}(e'')^\dagger, \hat{V}_v\right]\right) \qquad \text{(V.59)}\end{aligned}$$

and N_v is the value of lapse function N at $v \in \sigma$.

Deparametrisation with Gaussian Dust

Instead of dealing with vacuum GR, where one has to solve the scalar constraint $C[N]$, one can construct observables, e.g., by adding matter to the theory and trying to find local coordinates such that the constraint acquires the form $C = P + H$ in terms of the conjugated momentum P to the matter degree of freedom. If this form is achieved, one speaks of "relational observables" and "deparametrisation" [147–153]: the function H becomes a physical, conserved Hamiltonian density which drives the physical evolution of the observables with respect to the matter degree of freedom (which therefore plays the role of physical clock, τ). While not all types of matter allow for this decomposition, a possible choice is Gaussian dust: in the framework of Torre and Kuchař [147], the Lagrangian added to the Einstein-Hilbert action describing Gaussian dust is

$$\mathcal{L}_{GD} = -\sqrt{|\det(g)|}\left(\frac{\varrho}{2}(g^{\mu\nu}T_{,\mu}T_{,\nu} + 1) + g^{\mu\nu}T_{,\mu}(W_j S^j_{,\nu})\right) \tag{V.60}$$

with the fields ϱ and W_j having dimension cm^{-4}, while the fields T and S^j have dimension cm. Performing Legendre transformation, one can show that the time-evolution of an observable O_F (associated with phase space function F) is encoded as the Schrödinger-like equation $dO_F(\tau)/d\tau = \{H, O_F(\tau)\}$, where

$$H = C[1] = \int dx^3 C(x) \tag{V.61}$$

is for this reason called the *true Hamiltonian*. We see that C is no longer a constraint whose vanishing must be imposed, but in fact it generates time-translations. Thus, if one takes this viewpoint, the quantum scalar constraint presented above is understood as the quantum operator producing the dynamics of geometric degrees of freedom with respect to the classical observer provided by the dust.

V.C Cosmological Coherent States Expectation Values

In this section we will quote the work from [132, 133] by focussing on a subfamily of the coherent states $\Psi^t_{\gamma,\{h^{\mathbb{C}}\}}$, which we claim to be suited to describe flat Robertson-Walker geometries at a given instance, i.e. on the spatial manifold σ. The question of whether these states are actually stable under the dynamics is still open and will not be addressed here.

V.C.1 Choice of States

We follow [133] and introduce an infrared cut-off by restricting the spatial manifold σ to a compact submanifold, σ_R, which we equip with the topology of a 3-torus, that is, periodic boundary conditions. With respect to a fiducial metric η we identify R as the coordinate length of the torus, which in principle allows us to remove the cut-off by sending $R \to \infty$. Thus, we are interested in a fixed graph γ, which is chosen to be a the cubic lattice $\mathbb{Z}^3_{\mathcal{N}}$ embedded in σ_R for some finite $\mathcal{N} \in \mathbb{N}$. As such, we shall only consider a subalgebra of the holonomy-flux algebra: the holonomies along the edges of γ and the fluxes across the surfaces of a dual cell-complex.

The three directions of the lattice can be chosen adapted to the fiducial metric η, so that the coordinate length of a side of the lattice is R. On the other hand, due to σ_R being compact, γ has a finite number of vertices, $\mathcal{N}^3$. Assuming the lattice to be regular with respect to η, we therefore find that the coordinate distance between two neighbouring vertices is $\mu := R/\mathcal{N}$.
Now, we remember the calculations (IV.192),(IV.224) and (IV.233): the classical geometry that we want to reproduce is described by a line element that, in these coordinates, reads

$$ds^2 = -N^2 dt^2 + a^2(dx^2 + dy^2 + dz^2) \tag{V.62}$$

with N the lapse function and a the scale factor encoding the spatial geometry. In Ashtekar-Barbero variables, we find for the connection and densitised triad respectively

$$A^I_a = c\delta^I_a, \qquad E^a_I = p\delta^a_I \tag{V.63}$$

with c and p being the fundamental variables. One can now compute the holonomy and the flux along each edge e_I in direction I:

$$h(e_I) = e^{-c\mu\tau_I}, \qquad E^J(S_{e_I}) = p\mu^2 n^J_{(I)} \tag{V.64}$$

where $\vec{n}_{(I)}$ is the unit vector normal to S_{e_I} (so its components with respect to Cartesian coordinates are $n^J_{(I)} = \delta^J_I$). Therefore, according to (V.33), the element $H_I \in \mathrm{SL}(2,\mathbb{C})$ that should label the coherent state $\psi^t_{e_I,H_I} \in \mathcal{H}_{e_I}$ is (no sum over I)

$$\begin{aligned} H_I &= \exp\left(-\frac{it}{\hbar\kappa\beta} p\mu^2 \tau_I\right) e^{-c\mu\tau_I} = \exp\left[\left(-2c\mu - i\frac{2t}{\hbar\kappa\beta} p\mu^2\right) \vec{n}_{(I)} \cdot \vec{\tau}/2\right] = \\ &= n_I \exp\left[\left(-2\mu c - i\frac{2\mu^2 p}{\ell^2 \beta}\right) \tau_3/2\right] n_I^\dagger \end{aligned} \tag{V.65}$$

where in the third step we used the $SU(2)$-covariance of τ_I to move the rotation from its basis index to its matrix indices. In particular, n_I are the $SU(2)$ elements that rotate the unit vector $\hat{z}$ into the unit vector $\vec{n}_{(I)}$, and are explicitly given by

$$n_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \qquad n_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \qquad n_3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{V.66}$$

In this way, we have expressed H_I in its *holomorphic decomposition*, which for a generic $SL(2,\mathbb{C})$ element reads $n \exp(\bar{z}\tau_3/2) n'^\dagger$ for $z \in \mathbb{C}$ and $n, n' \in SU(2)$. While in general z, n and n' are independent, in this particularly simple case we find that $n = n'$ are fixed (though different for the three possible orientations of the edges) and we read off

$$z = -2\mu c + i\frac{2\mu^2 p}{\ell^2 \beta} \equiv \xi + i\eta \tag{V.67}$$

The complex number z is therefore the only label of our coherent states, encoding the classical geometry described by the canonical pair (c,p). In the derivation above the numerical values of c and p were computed using an *embedded lattice*. In the following, however, we will refer to an *abstract graph* whose label $z = \xi + i\eta$ is related to the numerical values c, p and μ according to (V.67).
Having the labels $\{h^{\mathbb{C}}\} = \{H\}$, we finally find our coherent states:

$$\begin{aligned} \Psi_{(c,p)}(\{g\}) &:= \prod_{e\in E(\gamma)} \psi^t_{e,h^{\mathbb{C}}_e}(g_e) = \prod_{I\in\{1,2,3\}} \prod_{k\in\mathbb{Z}^3_{\mathcal{N}}} \psi_{I,H_I}(g_{k,I}) \\ \psi_{I,H_I}(g) &:= \frac{1}{\sqrt{\langle 1\rangle_z}} \sum_{j\in\mathbb{N}/2} d_j e^{-j(j+1)t/2} \sum_{m=-j}^{j} e^{izm} D^{(j)}_{mm}(n_I^\dagger g n_I) \end{aligned} \tag{V.68}$$

where $\langle 1\rangle_z := ||\psi_{I,H_I}||^2$ is the normalisation of the state and again $\mathbb{Z}_{\mathcal{N}} = \{0, 1..., \mathcal{N}-1\}$.
These are states on the kinematical Hilbert space. As the next step, the implementation of the Gauss and diffeomorphism constraint does not require further work, as we have already seen that the they are both solved up to corrections of order t on the cosmological coherent states.

We conclude that the states introduced above can be considered as physical states. The remainder of the section collects some general results about this particular subfamily, which will be used in the following sections to perform computations. Because the extension to many edges is trivial, we can focus on a single edge, and therefore we shall drop the index 'I'. Moreover, we will sometimes write $H(z)$ to indicate that the $SL(2,\mathbb{C})$ label H effectively depends only on z given in (V.67).

V.C.2 General Properties of Cosmological Coherent States

Consider $\psi_{e,H(z)}(g)$ as in (V.68), with $H(z) = n e^{\bar{z}\tau_3/2} n^\dagger$ and $z = \xi + i\eta$ as in (V.67). The first result from [133] gives us a way to simplify expectation values of operators involving left-invariant vector fields.
In the following, we will change the basis of $\mathfrak{su}(2)$: instead of $I, J, K \in \{1, 2, 3\}$ we will consider the *spherical basis*, $s \in \{-1, 0, +1\}$, where $\tau_\pm := \mp(\tau_1 \pm i\tau_2)/\sqrt{2}$ and $\tau_0 := \tau_3$. The generators are thus

$$\tau_+ = i\sqrt{2}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \tau_- = -i\sqrt{2}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \tau_0 = -i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{V.69}$$

and satisfy the algebra $[\tau_+, \tau_-] = 2i\tau_0$, $[\tau_\pm, \tau_0] = \pm 2i\tau_\pm$.[13]

Lemma V.C.1. *Let $P(L, \hat{h})$ be a polynomial operator, with L^K the left-invariant vector field. Then:*

$$\langle \psi_{e,H(z)}, P(L(e), \hat{h}(e))\psi_{e,H(z)}\rangle = \langle \psi_{e,H(-z)}, P(-R(e), \hat{h}(e)^\dagger)\psi_{e,H(-z)}\rangle \tag{V.70}$$

Beweis. Because of linearity, if suffices to consider a single basis element $\hat{h}_{a_1b_1}(e)^{r_1} L^{K_1} .. \hat{h}_{a_nb_n}(e)^{r_n} L^{K_n}$ with $r_i \in \mathbb{N}_0$ and for arbitrary j, j' in the defintion of $\psi_{e,H(z)}$. We recall that $\hat{h}$ is a multiplication operator, while for R we find

$$\begin{aligned} R^K D^{(j)}_{ab}(g^\dagger) &= (-)^{b-a} R^K D^{(j)}_{-b-a}(g) = (-)^{b-a} \left.\frac{d}{ds}\right|_{s=0} D^{(j)}_{-b-a}(e^{s\tau_K} g) = \\ &= \left.\frac{d}{ds}\right|_{s=0} D^{(j)}_{ab}((e^{s\tau_K} g)^\dagger) = \left.\frac{d}{ds}\right|_{s=0} D^{(j)}_{ab}(g^\dagger e^{-s\tau_K}) = -\left.\frac{d}{ds}\right|_{s=0} D^{(j)}_{ab}(g^\dagger e^{s\tau_K}) \end{aligned} \tag{V.71}$$

obtained using the properties of Wigner matrices. In light of this, we have

$$\begin{aligned} &\int d\mu_H(g)\overline{D^{(j')}_{m'n'}(n^\dagger g n)} D^{(\frac{1}{2})}_{a_1b_1}(g)^{r_1} L^{K_1} \ldots D^{(\frac{1}{2})}_{a_nb_n}(g)^{r_n} L^{K_n} D^{(j)}_{mn}(n^\dagger g n)\delta_{m'n'}\delta_{mn} e^{izm} e^{-i\bar{z}m'} = \\ &= \left.\frac{d}{ds_1}\right|_{s_1=0} \cdots \left.\frac{d}{ds_n}\right|_{s_n=0} \int d\mu_H(g)\overline{D^{(j')}_{m'm'}(n^\dagger g n)} D^{(\frac{1}{2})}_{a_1b_1}(g)^{r_1} D^{(\frac{1}{2})}_{a_2b_2}(g e^{s_1\tau_{K_1}})^{r_2} \times \\ &\quad \times D^{(\frac{1}{2})}_{a_nb_n}(g e^{s_1\tau_{K_1}} \ldots e^{s_{n-1}\tau_{K_{n-1}}})^{r_n} D^{(j)}_{mm}(n^\dagger g^\dagger e^{s_1\tau_{K_n}} n) e^{izm} e^{-i\bar{z}m} = \\ &= (-1)^n \int d\mu_H(g^\dagger)\overline{D^{(j')}_{m'm'}(n^\dagger g^\dagger n)} D^{(\frac{1}{2})}_{a_1b_1}(g^\dagger)^{r_1} R^{K_1} \ldots D^{(\frac{1}{2})}_{a_nb_n}(g^\dagger)^{r_n} R^{K_n} D^{(j)}_{mm}(n^\dagger g^\dagger n) e^{izm} e^{-i\bar{z}m'} = \\ &= (-1)^n \int d\mu_H(g)\overline{D^{(j')}_{-m'-m'}(n^\dagger g n)} D^{(\frac{1}{2})}_{a_1b_1}(g^\dagger)^{r_1} \ldots D^{(\frac{1}{2})}_{a_nb_n}(g^\dagger)^{r_n} R^{K_n} D^{(j)}_{-m-m}(n^\dagger g n) e^{izm} e^{-i\bar{z}m'} = \\ &= (-1)^n \int d\mu_H(g)\overline{D^{(j')}_{m'm'}(n^\dagger g n)} D^{(\frac{1}{2})}_{a_1b_1}(g^\dagger) R^{K_1} \ldots D^{(\frac{1}{2})}_{a_nb_n}(g^\dagger)^{r_n} R^{K_n} D^{(j)}_{mm}(n^\dagger g n) e^{i(-z)m} e^{-i(-\bar{z})m'} \end{aligned} \tag{V.72}$$

where in the second step we renamed the integration variable $g \to g^\dagger$ and made use of (V.71), in the third step we used $d\mu_H(g) = d\mu_H(g^\dagger)$ and $D^{(j)}_{mn}(g^\dagger) = \overline{D^{(j)}_{nm}(g)} = (-1)^{n-m} D^{(j)}_{-n-m}(g)$, and in the last we renamed $-m \to m, -m' \to m'$ (recall that sums over such indices are understood). This gives the statement. □

[13] This does not change the action of geometric operators such as volume (V.50), since they are by construction $SU(2)$-scalars, and hence invariant under any basis transformation.

Lemma V.C.2. *Let $M(R(e),\hat{h}(e))^{K_1,\ldots,K_n}_{a_1b_1,\ldots,a_{n'}b_{n'}}$ be a monomial operator, with index-structure stemming from $R^{K_i}(e)$ and $\hat{h}_{a_ib_i}(e)$. Then:*

$$\begin{aligned}&\langle\psi_{e,H(z)},P(R(e),\hat{h}(e))^{K_1,\ldots,K_n}_{a_1b_1,\ldots,a_{n'}b_{n'}}\psi_{e,H(z)}\rangle=D^{(1)}_{-K_1,-S_1}(n)\ldots D^{(1)}_{-K_n,-S_n}(n)\times\\&\times D^{(\frac12)}_{a_1a_1'}(n)D^{(\frac12)}_{b_1'b_1}(n^\dagger)\ldots D^{(\frac12)}_{a_{n'}a'_{n'}}(n)D^{(\frac12)}_{b'_{n'}b_{n'}}(n^\dagger)\langle\psi_{e,H(z)|_{n=n_3}},P(R(e),\hat{h}(e))^{S_1,\ldots,S_n}_{a_1'b_1',\ldots,a'_{n'}b'_{n'}}\psi_{e,H(z)|_{n=n_3}}\rangle\end{aligned}\tag{V.73}$$

where we point out that $H(z)|_{n=n_3}=e^{z\tau_3/2}$.

Beweis. First, consider the action of R^K on $D^{(j)}_{mn}(n^\dagger gn)$:

$$\begin{aligned}R^KD^{(j)}_{mn}(n^\dagger gn)&=D^{(j)}_{mm'}(n^\dagger)\left(R^KD^{(j)}_{m'n'}(g)\right)D^{(j)}_{n'n}(n)=D^{(j)}_{mm'}(n^\dagger)D'^{(j)}_{m'\mu}(\tau_K)D^{(j)}_{\mu n'}(g)D^{(j)}_{n'n}(n)=\\&=D^{(j)}_{mm'}(n^\dagger)D'^{(j)}_{m'\mu}(\tau_K)D^{(j)}_{\mu\nu}(n)D^{(j)}_{\nu n}(n^\dagger gn)=\\&=D^{(1)}_{-K-S}(n)D'^{(j)}_{m\nu}(\tau_S)D^{(j)}_{\nu n}(n^\dagger gn)\end{aligned}\tag{V.74}$$

where in the last step we used that

$$\sum_{m',n'}D^{(j)}_{mm'}(g^\dagger)D'^{(j)}_{m'n'}(\tau_K)D^{(j)}_{n'n}(g)=\sum_L D^{(1)}_{-K-L}(g)D'^{(j)}_{mn}(\tau_L)\tag{V.75}$$

Hence, for the generic monomial, we express numerous times the product of two holonomies as a linear combination with fixed coefficients c:

$$\begin{aligned}&\int d\mu_H(g)\overline{D^{(j')}_{m'n'}(n^\dagger gn)}\hat{h}_{a_1b_1}...R^{K_n}D^{(j)}_{mn}(n^\dagger gn)=\\&=D^{(\frac12)}_{a_1a_1'}(n)D^{(\frac12)}_{b_1'b_1}(n^\dagger)...D^{(\frac12)}_{a_na_n'}(n)D^{(\frac12)}_{b_n'b_n}(n^\dagger)\int d\mu_H(g)\overline{D^{(j')}_{m'n'}(n^\dagger gn)}\times\\&\quad\times D^{(\frac12)}_{a_1'b_1'}(n^\dagger gn)R^{K_1}...D^{(\frac12)}_{a_n'b_n'}(n^\dagger gn)\left(D^1_{-K_n-S_n}(n)D'^{j}_{m\mu_n}(\tau_{S_n})D^{(j)}_{\mu_nn}(n^\dagger gn)\right)=\end{aligned}\tag{V.76}$$

$$\begin{aligned}&=D^{(\frac12)}_{a_1a_1'}(n)D^{(\frac12)}_{b_1'b_1}(n^\dagger)...D^{(\frac12)}_{a_na_n'}(n)D^{(\frac12)}_{b_n'b_n}(n^\dagger)D^1_{-K_n-S_n}(n)D'^{j}_{m\mu_n}(\tau_{S_n})\times\\&\quad\times\int d\mu_H(g)\overline{D^{(j')}_{m'n'}(n^\dagger gn)}D^{(\frac12)}_{a_1'b_1'}(n^\dagger gn)R^{K_1}...R^{K_{n-1}}\sum_{j_n}c^n_{j_n,\mu_n'\nu_n}(\mu_n)D^{j_n}_{\mu_n'\nu_n'}(n^\dagger gn)=\\&=D^{(\frac12)}_{a_1a_1'}(n)D^{(\frac12)}_{b_1'b_1}(n^\dagger)...D^{(\frac12)}_{a_na_n'}(n)D^{(\frac12)}_{b_n'b_n}(n^\dagger)D^1_{-K_n-S_n}(n)...D^1_{-K_1-S_1}(n)\times\\&\quad\times\left(D'^{j}_{m\mu_n}(\tau_{S_n})...D'^{j}_{m\mu_1}(\tau_{S_1})\times\int d\mu_H(g)\overline{D^{(j')}_{m'n'}(g)}\sum_{j_n\ldots j_1}c^1_{j_1,\mu_1',\nu_1}(\mu_1)...c^n_{j_n,\mu_n'\nu_n}(\mu_n)D^{j_1}_{\mu_1'\nu_1'}(g)\right)\end{aligned}$$

where in the last line we used invariance of the Haar measure to replace $n^\dagger gn\to g$. We now see that the term in brackets is nothing but the expansion of $\int d\mu_H(g)\overline{D^{(j')}_{m'n'}(g)}\hat{h}_{a_1b_1}...R^{K_n}D^{(j)}_{mn}(g)$, which was the statement. □

Lemma V.C.3. *Let $P(R,L,\hat{h})$ be a polynomial operator on $\mathcal{H}_e$. Then upon identifying the $su(2)$ label K with the numbers $0,\pm1$:*

$$\begin{aligned}\langle\psi_{e,H(z)|_{n=n_3}},P(R,L,\hat{h})L^K\psi_{e,H(z)|_{n=n_3}}\rangle&=e^{-izK}\langle\psi_{e,H(z)|_{n=n_3}},P(R,L,\hat{h})R^K\psi_{e,H(z)|_{n=n_3}}\rangle\\\langle\psi_{e,H(z)|_{n=n_3}},L^KP(R,L,\hat{h})\psi_{e,H(z)|_{n=n_3}}\rangle&=e^{-i\bar{z}K}\langle\psi_{e,H(z)|_{n=n_3}},R^KP(R,L,\hat{h})\psi_{e,H(z)|_{n=n_3}}\rangle\end{aligned}\tag{V.77}$$

Beweis. Since $D'^{j}_{mn}(\tau_K)$ enforces $n+K-m=0$, one gets

$$\begin{aligned}L^KD^{(j)}_{mm}e^{izm}&=D^{(j)}_{m\mu}(g)D'^{(j)}_{\mu m}(\tau_K)e^{izm}=e^{-izK}D^{(j)}_{\mu m}(g)D'^{(j)}_{m\mu}(\tau_K)e^{izm}=\\&=e^{-izK}R^KD^{(j)}_{mm}(g)e^{izm}\end{aligned}\tag{V.78}$$

where in the second step we exchanged the dummy indices $\mu \leftrightarrow m$. This is the first property. For the second, we expand $P(R,L,\hat{h})\psi = \sum_j c_{jmn} D^{(j)}_{mn}(g)$ with some coefficients c:

$$\begin{aligned}
&\sum_j c_{jmn} \int d\mu_H(g) \overline{D^{(j')}_{m'm'}(g)} e^{-i\bar{z}m'} L^K D^j_{mn}(g) = \frac{1}{d_{j'}} c_{j'm'n} e^{-i\bar{z}m'} D'^{j'}_{m'n}(\tau_K) = \\
&= e^{-i\bar{z}K} \frac{1}{d_{j'}} c_{j'nm'} e^{-i\bar{z}m'} D'^{(j')}_{nm'}(\tau_K) = \\
&= e^{-i\bar{z}K} \sum_j c_{jn\mu} e^{-i\bar{z}m'} D'^{j}_{n\nu}(\tau_K) \int d\mu_H(g) \overline{D^{(j')}_{m'm'}(g)} D^j_{\nu\mu}(g) = \\
&= e^{-i\bar{z}K} R^K P(R,L,\hat{h})\psi
\end{aligned} \tag{V.79}$$

having exchanged the dummy indices $m' \leftrightarrow n$ in the second step. □

Now, if one uses both relation in (V.77), and the fact that $[R^K(e), L^M(e)] = 0$, one gets immediately the following result.

Corollary V.C.1. *The following cyclic property holds:*

$$\langle \psi_{e,H(z)|_{n=n_3}}, R^{K_1}..R^{K_n} \psi_{e,H(z)|_{n=n_3}} \rangle = e^{-2\eta K_n} \langle \psi_{e,H(z)|_{n=n_3}}, R^{K_n} R^{K_1}..R^{K_{n-1}} \psi_{e,H(z)|_{n=n_3}} \rangle \tag{V.80}$$

where $z = \xi + i\eta$.

As we will see in the next section, this property allows to greatly simplify the computations for the expectation value of any product of R's.

V.C.3 Expectation Values of Monomials on a Single Edge

In this section we will cite the computations of expectation values of the various monomials which appear in the geometric operators from [133]. As on a given edge e we have $\hat{E}^K(S_e) = -it\beta/4\ R^K(e)$ computing the expectation value of $R^K(e)$ is supposed to give us at leading order a factor t^{-1}. Hence, for a monomial to the N-th power in $\hat{E}(S_e)$ we will neglect all contributions of order $t^{-(N-2)}$ when computing the expectation value of N many $R(e)$.
Moreover, thanks to lemma 2, it suffices to express everything on cosmological coherent states with $H(z)|_{n=n_3}$, and so we will use a shorthand notation for the *non normalised* expectation values:

$$\langle P(R(e), \hat{h}(e)) \rangle_z := \langle 1 \rangle_z \langle \psi_{e,H(z)|_{n=n_3}}, P(R(e), \hat{h}(e)) \psi_{e,H(z)|_{n=n_3}} \rangle \tag{V.81}$$

where $\langle 1 \rangle_z := ||\psi_{I,H_I}||^2$ is the normalisation of the state, which will be computed in the following subsection.

Monomials of right-invariant Vector Field

Consider first N right-invariant vector fields, all with magnetic index $s_1 = .. = s_N = 0$. We have

$$\begin{aligned}
&\langle R^{s_1}..R^{s_N} \rangle_z = \\
&= \sum_{j,j'} d_j d_{j'} e^{-j(j+1)t/2} e^{-j'(j'+1)t/2} e^{-i\bar{z}m'} e^{izm} \int d\mu_H(g) \overline{D^{(j')}_{m'm'}(g)} D'^{(j)}_{m\mu_N}(\tau_0)..D'^{(j)}_{\mu_2\mu_1}(\tau_0) D^{(j)}_{\mu_1 m}(g) \\
&= \sum_{j,j'} d_j d_{j'} e^{-j(j+1)t/2 - j'(j'+1)t/2} (-2im)^N e^{-i\bar{z}m'} e^{izm} \int d\mu_H(g) \overline{D^{(j')}_{m'm'}(g)} D^{(j)}_{mm}(g) \\
&= \sum_j d_j e^{-j(j+1)t} (-2im)^N e^{-2\eta m} = \sum_j d_j e^{-j(j+1)t} (i\partial_\eta)^N e^{-2\eta m} = \\
&= (i\partial_\eta)^N \sum_j d_j e^{-j(j+1)t} \frac{\sinh(d_j\eta)}{\sinh(\eta)} = (i\partial_\eta)^N \langle 1 \rangle_z
\end{aligned} \tag{V.82}$$

where we used $D'_{mn}(\tau_0) = -2im\delta_{mn}$ in the second step and the geometric sum $\sum_{m=-j}^{j} e^{-2\eta m} = \sinh(d_j\eta)/\sinh(\eta)$ to go to the last line. It remains to compute $\langle 1 \rangle_z$, the normalisation of the state, for which we follow closely [154–156]. As the authors there have pointed out, this sum can be approximated after using the elementary

Poisson Summation Formula III.C.1.

By realizing that for $d_j = 2j+1$ the term in the sum is even, we extend the sum to negative values, thus bringing $\langle 1\rangle_z$ in the form to apply this theorem:

$$\begin{aligned}\langle 1\rangle_z &= \sum_{d_j=1}^{\infty} d_j e^{-(d_j^2-1)t/4}\frac{\sinh(d_j\eta)}{\sinh(\eta)} = \frac{1}{2}\sum_{n=-\infty}^{\infty} n e^{-(n^2-1)t/4}\frac{\sinh(n\eta)}{\sinh(\eta)} = \\ &= \frac{1}{2}\int_{\mathbb{R}} du \sum_{n\in\mathbb{Z}} e^{-i2\pi n u} e^{-tu^2/4} e^{t/4} u \frac{\sinh(u\eta)}{\sinh(\eta)} \end{aligned} \tag{V.83}$$

Upon completing the square, in the exponential one gets the term $e^{-4\pi^2 n^2/t}$ which, for $t\to 0$, goes to 0 faster than any polynomial, unless $n=0$. We conclude that, for $1 \gg t$, only the $n=0$ term of the sum contributes, up to an error of order $\mathcal{O}(t^\infty)$. We thus find

$$\langle 1\rangle_z = \frac{1}{2}e^{t/4}\int_{\mathbb{R}} du\ u e^{-tu^2/4}\frac{e^{2\eta u}}{\sinh(\eta)} = 2e^{t/4}\sqrt{\frac{\pi}{t^3}}\frac{\eta e^{\eta^2/t}}{\sinh(\eta)} \tag{V.84}$$

Because of the factor $e^{\eta^2/t}$ in $\langle 1\rangle_z$, the leading order of (V.82) in t is obtained when all N derivatives ∂_η hit $e^{\eta^2/t}$, giving $\mathcal{O}(1/t^N)$.
Let us now consider the case where some indices $s_1,...,s_n$ are not equal to zero. Since $D'^{(j)}_{\mu_{i+1}\mu_i}(\tau_{s_i})$ implies $\mu_{i+1} = \mu_i + s_i$ and we have $\mu_0 = \mu_{N+1} = m$ it follows that $\sum_i s_i = 0$. Consequently, a single non-vanishing s_i is impossible: we shall therefore consider a pair s_1, s_2 with opposite sign. Moreover, we will neglect all contributions smaller than $\mathcal{O}(1/t^{N-1})$, since we saw that the leading order (for (V.82)) is $\sim 1/t^N$. Using the algebra (for $s_1, s_2, s \neq 0$)

$$[R^{s_1}, R^{s_2}] = -i(s_1-s_2)R^0, \qquad [R^s, R^0] = -2isR^s \tag{V.85}$$

we find for the expectation value with a spacing C between s_1 and s_2

$$\begin{aligned}\langle R^0...R^{s_1}\overbrace{R^0...R^0}^{C}R^{s_2}...R^0\rangle_z &= \langle R^0...R^0 R^{s_1}R^0...R^0R^{s_2}\rangle_z = \\ &= \langle\overbrace{R^0...R^0}^{N-2}R^{s_1}R^{s_2}\rangle_z - 2iCs_2\langle\overbrace{R^0...R^0}^{N-3}R^{s_1}R^{s_2}\rangle_z + \mathcal{O}(1/t^{N-2}) = \\ &= \left((i\partial_\eta)^{N-2} - 2iCs_2(i\partial_\eta)^{N-3}\right)\langle R^{s_1}R^{s_2}\rangle_z + \mathcal{O}(1/t^{N-2})\end{aligned} \tag{V.86}$$

having used (V.80) in the first step and (V.85) in the second. We reduced the problem to evaluating the expectation value $\langle R^{s_1}R^{s_2}\rangle_z$. But this can be done without effort by combining the cyclicity property and the algebra: it is

$$\begin{aligned}\langle R^{s_1}R^{s_2}\rangle_z &= e^{-2\eta s_2}\langle R^{s_2}R^{s_1}\rangle_z = e^{-2\eta s_2}(\langle R^{s_1}R^{s_2}\rangle_z - \langle[R^{s_1},R^{s_2}]\rangle_z) = \\ &= e^{-2\eta s_2}\langle R^{s_1}R^{s_2}\rangle_z + e^{-2\eta s_2} i(s_1-s_2)\langle R^0\rangle_z = \\ &= e^{-2\eta s_2}\langle R^{s_1}R^{s_2}\rangle_z - e^{-2\eta s_2}(s_1-s_2)\partial_\eta\langle 1\rangle_z\end{aligned} \tag{V.87}$$

which, solved for $\langle R^{s_1}R^{s_2}\rangle_z$, gives

$$\langle R^{s_1}R^{s_2}\rangle_z = \frac{e^{-\eta s_2}}{\sinh(\eta)}\partial_\eta\langle 1\rangle_z \tag{V.88}$$

Again, the leading order is obtained when all ∂_η hit $e^{\eta^2/t}$. It follows that the term proportional to C in (V.86) is negligible, and the other is already next-to-leading with respect to (V.82). Explicitly, we get

$$\langle R^0...R^{s_1}\overbrace{R^0...R^0}^{C}R^{s_2}...R^0\rangle_z = -i\frac{e^{-\eta s_2}}{\sinh(\eta)}(i\partial_\eta)^{N-1}\langle 1\rangle_z + \mathcal{O}(1/t^{N-2}) \tag{V.89}$$

A similar calculation reveals that four and more non-vanishing indices are of order $\mathcal{O}(1/t^{N-2})$, and will thus be neglected.

The final result up to linear quantum corrections thus reads:

$$\langle R^{s_1}\dots R^{s_N}\rangle_z = \tag{V.90}$$
$$= \left[\delta_0^{s_1\dots s_N}(i\partial_\eta)^N - \frac{i}{\sinh(\eta)}\sum_{A<B=1}^{N}\delta_0^{s_1..\not{s}_A..\not{s}_B..s_N}\left(\delta_{+1-1}^{s_A s_B}e^{+\eta}+\delta_{-1+1}^{s_A s_B}e^{-\eta}\right)(i\partial_\eta)^{N-1}\right]\langle 1\rangle_z$$

where we defined $\delta_0^{s_1\dots s_N} := \delta_0^{s_1}\dots\delta_0^{s_N}$. Making use of lemma 1, equation (V.70), one can straightforwardly generalise this result to a monomial in left-invariant vector fields:

$$\begin{aligned}\langle L^{s_1}\dots L^{s_N}\rangle_z = (-1)^N\langle R^{s_1}\dots R^{s_N}\rangle_{-z} = (-1)^{2N}\langle R^{s_N}\dots R^{s_1}\rangle_z = \\ = \langle R^{s_N}\dots R^{s_1}\rangle_z\end{aligned} \tag{V.91}$$

where in the second step we used the explicit expression (V.90) to find how a change in sign of z (or η) influences the expectation value.

Monomials of Holonomy Operator

As is well known from recoupling theory, the product of Wigner matrices can be expressed as a linear combination of a single Wigner matrix [291]:

$$D_{ab}^{(j_1)}(g)D_{cd}^{(j_2)}(g) = \sum_{j=|j_1-j_2|}^{j_1+j_2} d_j(-1)^{m-n}\begin{pmatrix} j_1 & j_2 & j \\ a & c & m\end{pmatrix}\begin{pmatrix} j_1 & j_2 & j \\ b & d & n\end{pmatrix}D_{-m-n}^{(j)}(g) \tag{V.92}$$

This property is extremely useful, since it allows to reduce the problem of computing $\langle\hat{h}_{a_1b_1}\dots\hat{h}_{a_nb_n}\rangle_z$ to computing $\langle\hat{h}_{mn}^{(j)}\rangle_z$ (for the required values of j), by which we mean the operator whose action is to multiply by $D_{mn}^{(j)}(g)$.
From the explicit expression (V.68), we obtain (without normalisation)

$$\begin{aligned}\langle\hat{h}_{ab}^{(k)}\rangle_z &= \sum_{j,j'} d_j d_{j'} e^{-[j(j+1)+j'(j'+1)]t/2} e^{i(zm-\bar{z}m')}\int d\mu_H(g)\overline{D_{m'm'}^{(j')}(g)}D_{ab}^{(k)}(g)D_{mm}^{(j)}(g) = \\ &= \sum_{j,j'} d_j d_{j'} e^{-[j(j+1)+j'(j'+1)]t/2} e^{i\xi(m-m')}e^{-\eta(m+m')}\begin{pmatrix} j & k & j' \\ m & a & -m'\end{pmatrix}\begin{pmatrix} j & k & j' \\ m & b & -m'\end{pmatrix} = \\ &= \delta_{ab}e^{-i\xi a}\gamma_a^k\end{aligned} \tag{V.93}$$

where in the second line we performed the integral, and in the third we used the observation that $a = m'-m = b$ to extract $e^{i\xi(m-m')} = e^{-i\xi a}$ from the sums and defined the quantity

$$\gamma_a^k := \sum_{j,j'} d_j d_{j'} e^{-t[j(j+1)+j'(j'+1)]/2} e^{-\eta(m+m')}\begin{pmatrix} k & j & j' \\ a & m & -m'\end{pmatrix}^2 \tag{V.94}$$

If we interchange in γ_a^k the contracted indices $j \leftrightarrow j'$, $m \leftrightarrow m'$ everything is clearly invariant except for the $3j$-symbol:

$$\begin{pmatrix} k & j & j' \\ a & m & -m'\end{pmatrix} \to \begin{pmatrix} k & j' & j \\ a & m' & -m\end{pmatrix} = \begin{pmatrix} k & j & j' \\ -a & m & -m'\end{pmatrix} \tag{V.95}$$

As the index a appeared only in the $3j$-symbol this leads to $\gamma_a^k \to \gamma_{-a}^k$, but since we only interchanged contracted indices γ_a^k must stay invariant: we conclude that

$$\gamma_a^k = \gamma_{-a}^k \tag{V.96}$$

The various values of γ_a^k can now be computed with the Poisson Summation Formula. In paper [133] the explicit computations are presented for $k = 1/2$ and $k = 1$ (which are sufficient for the Hamiltonian operator).

The results are:

$$\begin{aligned}\gamma^{1/2}_{1/2} &= \langle 1\rangle_z \left[1+\frac{t}{4\eta}\left(\frac{3}{4}\eta-\tanh\left(\frac{\eta}{2}\right)\right)+\mathcal{O}(t^2)\right]\\ \gamma^{1}_{0} &= \langle 1\rangle_z \left[1+t\frac{2\sinh(\eta/2)}{\eta\sinh(\eta)}+\mathcal{O}(t^2)\right]\\ \gamma^{1}_{1} &= \langle 1\rangle_z \left[1-t\left(\frac{1}{4}+\frac{1}{2\eta}\tanh(\eta/2)\right)+\mathcal{O}(t^2)\right]\end{aligned} \tag{V.97}$$

Holonomies and right-invariant Vector Fields

In this section we present the strategy to compute expectation values of monomials involving both holonomies and right-invariant vector fields. We consider a couple of explicit examples.
Let us start with the commutator of a holonomy with N right invariant vector fields. Using the algebra (V.21) and dropping all terms of order $\mathcal{O}(1/t^{N-3})$ and lower (since the leading order is $\mathcal{O}(1/t^{N-1})$), we find

$$\begin{aligned}&\langle \hat{h}_{ac}[\hat{h}^\dagger_{cb}, R^{s_1}...R^{s_N}]\rangle_z = \delta_{ac}\langle R^{s_1}...R^{s_N}\rangle_z - \langle \hat{h}_{ab}R^{s_1}...R^{s_N}\hat{h}^\dagger_{cb}\rangle_z =\\ &= \delta_{ab}\langle R^{s_1}...R^{s_N}\rangle_z - \langle R^{s_1}\hat{h}_{ac}R^{s_2}...R^{s_N}\hat{h}^\dagger_{cb}\rangle_z + D'^{(1/2)}_{ad}(\tau_{s_1})\langle \hat{h}_{dc}R^{s_2}...R^{s_N}\hat{h}^\dagger_{cb}\rangle_z =\\ &= \delta_{ab}\langle R^{s_1}...R^{s_N}\rangle_z - \langle R^{s_1}R^{s_2}\hat{h}_{ac}...R^{s_N}\hat{h}^\dagger_{cb}\rangle_z + D'^{(1/2)}_{ad}(\tau_{s_2})\langle R^{s_1}\hat{h}_{dc}R^{s_3}...R^{s_N}\hat{h}^\dagger_{cb}\rangle_z +\\ &+ D'^{(1/2)}_{ad}(\tau_{s_1})\langle R^{s_2}\hat{h}_{dc}R^{s_3}...R^{s_N}\hat{h}^\dagger_{cb}\rangle_z - D'^{(1/2)}_{ae}(\tau_{s_1})D'^{(1/2)}_{ed}(\tau_{s_2})\langle \hat{h}_{dc}R^{s_3}...\hat{h}^\dagger_{cb}\rangle_z = ... =\\ &= \sum_{A=1}^{N} D'^{(\frac{1}{2})}_{ab}(\tau_{s_A})\langle R^{s_1}...\not{R}^{s_A}...R^{s_N}\rangle_z -\\ &- \sum_{A<B=1}^{N} D'^{(\frac{1}{2})}_{ac}(\tau_{s_A})D'^{(\frac{1}{2})}_{cb}(\tau_{s_B})\langle R^{s_1}...\not{R}^{s_A}...\not{R}^{s_B}...R^{s_N}\rangle_z + \mathcal{O}(1/t^{N-3})\end{aligned} \tag{V.98}$$

So, such term can be brought back to the expectation values of R's only.
The other type of mixed term is of the form $\hat{h}_{ab}R^{s_1}...R^{s_N}$. From expression (V.68), we get (without normalisation)

$$\begin{aligned}\langle \hat{h}_{ab}R^{s_1}...R^{s_N}\rangle_z &= e^{-i\bar{z}b}\sum_{j,j'} d_j d_{j'} e^{-t[j(j+1)+j'(j'+1)]/2}\times \\ &\times D'^{(j)}_{m\mu_N}(\tau_{s_N})...D'^{(j)}_{\mu_2\mu_1}(\tau_{s_1})\begin{pmatrix}\frac{1}{2} & j & j'\\ a & \mu_1 & -m'\end{pmatrix}\begin{pmatrix}\frac{1}{2} & j & j'\\ b & m & -m'\end{pmatrix}e^{-2\eta m}\end{aligned} \tag{V.99}$$

where we again used (V.92) and performed the group integral. As we did previously for monomials in R's, let us consider the case $s_1 = ... = s_N = 0$ first. Using $D'^{(j)}_{mn}(\tau_0) = -2im\delta_{mn}$, it is easy to see that

$$\langle \hat{h}_{ab}R^0\dots R^0\rangle_z = e^{-\eta b}(i\partial_\eta)^N e^{\eta b}\langle \hat{h}_{ab}\rangle_z \tag{V.100}$$

which has leading order $\mathcal{O}(1/t^N)$. Next, we have the possibility of a single index being nonzero, as well as a pair. The order of these is next-to-leading with respect to (V.100). Indeed, using $[R^0, R^s] = 2isR^s$ for $C \le N$, we get

$$\begin{aligned}\langle \hat{h}_{ab}\overbrace{R^0...R^0}^{C}R^s\overbrace{R^0...R^0}^{N-1-C}\rangle_z &= \langle \hat{h}_{ab}\overbrace{R^0...R^0}^{C-1}R^s\overbrace{R^0...R^0}^{N-C}\rangle_z + 2i\langle \hat{h}_{ab}\overbrace{R^0...R^0}^{C-1}R^s\overbrace{R^0...R^0}^{N-1-C}\rangle_z =\\ &= \langle \hat{h}_{ab}R^s\overbrace{R^0...R^0}^{N-1}\rangle_z + \mathcal{O}(1/t^{N-2}) =\\ &= e^{-\eta b}(i\partial_\eta)^{N-1}e^{\eta b}\langle \hat{h}_{ab}R^s\rangle_z + \mathcal{O}(1/t^{N-2})\end{aligned} \tag{V.101}$$

and

$$\langle \hat{h}_{ab}R^0...R^0R^sR^0...R^0R^{s'}R^0...R^0\rangle_z = (i\partial_\eta)^{N-2}\langle \hat{h}_{ab}R^sR^{s'}\rangle_z + \mathcal{O}(1/t^{N-2}) \tag{V.102}$$

We thus reduced the problem to the evaluation of $\hat{h}_{ab}R^s$ and $\hat{h}_{ab}R^sR^{s'}$. Again, these can be computed by usefully combining the cyclicity of lemma 3 with the algebra:

$$\begin{aligned}\langle\hat{h}_{ab}R^s\rangle_z &= \langle R^s\hat{h}_{ab}\rangle_z - \langle[R^s,\hat{h}_{ab}]\rangle_z = e^{i\bar{z}s}\langle L^s\hat{h}_{ab}\rangle_z - D'^{(1/2)}_{ac}(\tau_s)\langle\hat{h}_{cb}\rangle_z = \\ &= e^{i\bar{z}s}\left(\langle\hat{h}_{ab}L^s\rangle_z + \langle[L^s,\hat{h}_{ab}]\rangle_z\right) - D'^{(1/2)}_{ac}(\tau_s)\langle\hat{h}_{cb}\rangle_z = \\ &= e^{i\bar{z}s}\left(e^{-izs}\langle\hat{h}_{ab}R^s\rangle_z + D'^{(1/2)}_{cb}(\tau_s)\langle\hat{h}_{ac}\rangle_z\right) - D'^{(1/2)}_{ac}(\tau_s)\langle\hat{h}_{cb}\rangle_z = \\ &= e^{2\eta s}\langle\hat{h}_{ab}R^s\rangle_z + e^{i\bar{z}s/2}\left(e^{i\bar{z}s/2}D'^{(1/2)}_{cb}(\tau_s)\langle\hat{h}_{ac}\rangle_z - e^{-i\bar{z}s/2}D'^{(1/2)}_{ac}(\tau_s)\langle\hat{h}_{cb}\rangle_z\right)\end{aligned} \tag{V.103}$$

leading to

$$\langle\hat{h}_{ab}R^s\rangle_z = \frac{se^{izs/2}}{2\sinh(\eta)}\left(e^{-i\bar{z}s/2}D'^{(1/2)}_{ac}(\tau_s)\langle\hat{h}_{cb}\rangle_z - e^{i\bar{z}s/2}\langle\hat{h}_{ac}\rangle_z D'^{(1/2)}_{cb}(\tau_s)\right) \tag{V.104}$$

A similar computation gives

$$\begin{aligned}\langle\hat{h}_{ab}R^sR^{s'}\rangle_z = &-i\frac{e^{\eta s}}{\sinh(\eta)}\langle\hat{h}_{ab}R^0\rangle_z + \\ &+\frac{s}{2\sinh(\eta)}e^{izs/2}\left(e^{-i\bar{z}s/2}D'^{(1/2)}_{ac}(\tau_s)\langle\hat{h}_{cb}R^{s'}\rangle_z - e^{i\bar{z}s/2}\langle\hat{h}_{ac}R^{s'}\rangle_z D'^{(1/2)}_{cb}(\tau_s)\right)\end{aligned} \tag{V.105}$$

Now, since (V.101) involves only $N-1$ derivatives of η, we can only get an $\mathcal{O}(1/t^{N-1})$ contribution if all derivatives hit $e^{\eta^2/t}$ in the normalisation appearing in $\langle\hat{h}_{ab}\rangle_z = \delta_{ab}e^{-i\xi a}\langle 1\rangle_z$ (which is correct at leading order).

Using the same argument for (V.102), and putting the results together with the $s_1 = ... = s_N = 0$ case, we finally obtain

$$\begin{aligned}\langle\hat{h}_{ab}R^{s_1}\dots R^{s_n}\rangle_z = \Big[&\delta_0^{s_1\dots s_N}\delta_{ac}e^{-\eta b}(i\partial_\eta)^N e^{\eta b} - \\ &-\frac{\sinh(\eta/2)}{\sinh(\eta)}\sum_{A=1}^N \delta_0^{s_1\dots\not{s}_A\dots s_N}(\delta^{s_A}_{+1}+\delta^{s_A}_{-1})e^{s_A\eta/2}D'^{(\frac{1}{2})}_{ac}(\tau^{s_A})(i\partial_\eta)^{N-1} - \\ &-i\frac{\delta_{ac}}{\sinh(\eta)}\sum_{A<B=1}^N \delta_0^{s_1\dots\not{s}_A\dots\not{s}_B\dots s_N}(\delta^{s_As_B}_{+1-1}+\delta^{s_As_B}_{-1+1})e^{s_A\eta}(i\partial_\eta)^{N-1}\Big]\langle\hat{h}_{cb}\rangle_z\end{aligned} \tag{V.106}$$

V.C.4 Expectation Values of the Volume Operator

The tools developed in the previous section shall now be exploited. We compute the expectation value of the volume following closely the computations from [133].

Thanks to (V.52), the expectation value of the Ashtekar-Lewandowski volume coincides with the expectation value of the $(k=1)$-Giesel-Thiemann volume operator (V.53) up to next-to-leading order in t. But to evaluate that, we only need the expectation values of $\hat{Q}^N_v$ for $N = 1, 2, 4$ and 6. Although these are operators on many edges, the expectation value reduces to the product of expectation values on each edge, so the only quantity we need is the expectation value of a string of N right-invariant vector fields. This was derived in (V.90), and restoring the dependence on $n \in SU(2)$, it reads

$$\begin{aligned}\langle\psi_{e,H(z)}, R^{k_1}..R^{k_N}\psi_{e,H(z)}\rangle = &\left(\frac{2\eta i}{t}\right)^N D^{(1)}_{-k_1-s_1}(n)..D^{(1)}_{-k_N-s_N}(n)\ (\delta_0^{s_1\dots s_N} + \\ &+\frac{t}{2\eta}[\delta_0^{s_1\dots s_N}\left(\frac{N(N+1)}{2\eta} - N\coth(\eta)\right) - \frac{1}{\sinh(\eta)}\sum_{A<B=1}^N \delta_0^{s_1..\not{s}_A..\not{s}_B\dots s_N}(\delta^{s_As_B}_{+1-1}+\delta^{s_As_B}_{-1+1})e^{s_A\eta}])\end{aligned} \tag{V.107}$$

In $\langle\hat{Q}^N_v\rangle$, one has a products of six such expectation values. The combinatorics is encoded in $\epsilon_{k_ik'_ik''_i}R^{k_i}(e_1)R^{k'_i}(e_2)R^{k''_i}(e_3)$, which motivates us to consider the object

$$\epsilon^{(n)}_{s_is'_is''_i} := \epsilon_{k_ik'_ik''_i}D^{(1)}_{-k_i-s_i}(n_1)D^{(1)}_{-k'_i-s'_i}(n_2)D^{(1)}_{-k'_i-s'_i}(n_3) \tag{V.108}$$

Since n_i are fixed $SU(2)$ elements, the components of this tensor can be computed explicitly using (V.66), and one fins in particular

$$\epsilon^{(n)}_{00s} = \delta_{s0} \tag{V.109}$$

This is enough for our purposes: indeed, we are interested only in corrections linear in t, which means that five of the six strings in the product must be comprised only of R's with zero index. $\epsilon^{(n)}_{00s}$ then forces the third index to be zero as well, so one obtains

$$\langle (R^0)^N\rangle_z = \delta_0^{s_1\ldots s_N}\left(\frac{2\eta i}{t}\right)^N\left[1+\frac{t}{2\eta}\left(\frac{N(N+1)}{2\eta}-N\coth(\eta)\right)\right] \tag{V.110}$$

that is, only the terms proportional to $\delta_0^{s_1..s_N}$ will contribute.

Now, the diffeomorphism-invariant quantity $\epsilon(e_a,e_b,e_c) := sgn(\det(a,b,c)) = sgn(abc)\epsilon_{abc}$ with $a,b,c\in\{1,2,3\}$ tells us that (calling $R^I_a := R^I(e_a)$)

$$\begin{aligned}
\langle\Psi_{(c,p)},\hat{Q}_v^N\Psi_{(c,p)}\rangle &= \langle\Psi_{(c,p)}, i^N\left(6\epsilon_{IJK}(R^I_1+R^I_{-1})(R^J_2+R^J_{-2})(R^K_3+R^K_{-3})\right)^N\Psi_{(c,p)}\rangle = \\
&= (6i)^N\prod_{i=1}^3\left(\sum_{n=0}^N\binom{N}{n}\langle(R^0_i)^n\rangle_z\langle(R^0_{-i})^{N-n}\rangle_z\right) = \\
&= (6i)^N\left(\sum_{n=0}^N\binom{N}{n}\langle(R^0)^n\rangle_z\langle(R^0)^{N-n}\rangle_z\right)^3 = \\
&= (6i)^N\left(\sum_{n=0}^N\binom{N}{n}\left(\frac{2\eta i}{t}\right)^N\left[1+\frac{t}{2\eta}\left(\frac{n(n+1)}{2\eta}-n\coth(\eta)\right)\right]\times\right.\\
&\quad\left.\times\left[1+\frac{t}{2\eta}\left(\frac{(N-n)(N-n+1)}{2\eta}-(N-n)\coth(\eta)\right)\right]\right)^3 = \\
&= (6i)^N\left(\frac{2\eta i}{t}\right)^{3N}\left[2^N+\frac{t}{2\eta^2}(N^2+3N)2^{N-2}-\frac{t}{2\eta}N2^N\coth(\eta)\right]^3
\end{aligned} \tag{V.111}$$

where we used

$$\sum_{n=0}^N\binom{N}{n} = 2^N,\qquad \sum_{n=0}^N\binom{N}{n}n = 2^{N-1}N,\qquad \sum_{n=0}^N\binom{N}{n}n^2 = (N+N^2)2^{N-2} \tag{V.112}$$

Thus, we get

$$\frac{\langle\Psi_{(c,p)},\hat{Q}_v^N\Psi_{(c,p)}\rangle}{\langle\Psi_{(c,p)},\hat{Q}_v\Psi_{(c,p)}\rangle^N} = 1+\frac{3t}{8\eta^2}N(N-1) \tag{V.113}$$

with which one can now compute the expectation value of the Giesel-Thiemann volume operator. For $k=1$, it reads

$$\begin{aligned}
\hat{V}^{GT}_{1,v} = &\frac{(\beta\hbar\kappa)^{\frac{3}{2}}}{2^5\sqrt{3}}\frac{\langle\Psi_{(c,p)},\hat{Q}_v\Psi_{(c,p)}\rangle^{1/2}}{128}\times \\
&\times\left[77\cdot\mathbb{1}+77\frac{\hat{Q}_v^2}{\langle\Psi_{(c,p)},\hat{Q}_v\Psi_{(c,p)}\rangle^2}-33\frac{\hat{Q}_v^4}{\langle\Psi_{(c,p)},\hat{Q}_v\Psi_{(c,p)}\rangle^4}+7\frac{\hat{Q}_v^6}{\langle\Psi_{(c,p)},\hat{Q}_v\Psi_{(c,p)}\rangle^6}\right]
\end{aligned} \tag{V.114}$$

so one finds (summing over all $\mathcal{N}^3$ vertices in the lattice)

$$\langle\Psi_{(c,p)},\hat{V}(\sigma)\Psi_{(c,p)}\rangle = \frac{(\beta\hbar\kappa)^{\frac{3}{2}}}{2^5\sqrt{3}}\mathcal{N}^3\sqrt{48}\left(\frac{2\eta}{t}\right)^{3/2}\left[1+\frac{3t}{4\eta^2}\left(\frac{7}{8}-\eta\coth(\eta)\right)+\mathcal{O}(t^2)\right] \tag{V.115}$$

Let us discuss this result (V.115): the state lives on an abstract graph, at which point ξ and η are some labels of the state. However, if we embed the graph in a manifold, these labels can be interpreted as the expectation values of holonomies and fluxes of the lattice (with μ being the coordinate length of a link). Specifically, they describe a (discrete) homogeneous and isotropic classical geometry, i.e. a flat Robertson-Walker metric (on a compactified torus). In particular, $\eta = \frac{2\mu^2 p}{\ell^2\beta}$ by (V.67). Consequently, the number $\mathcal{N}$ of all edges of a connected path along one direction is the fiducial torus length R over the spacing μ: $\mathcal{N} = R/\mu$. Hence, upon identifying the semi-classicality parameter $t=\hbar\kappa/\ell^2$, we find that at leading order the expectation value of the volume of the whole spatial slice reduces to (leaving η implicit in the next-to-leading order to ease the notation)

$$\langle\Psi_{(c,p)},\hat{V}(\sigma)\Psi_{(c,p)}\rangle = R^3p^{3/2}\left[1+\hbar\frac{3\kappa}{4\ell^2}\left(\frac{7}{8\eta^2}-\frac{1}{\eta}\coth(\eta)\right)+\mathcal{O}(\hbar^2)\right] \tag{V.116}$$

Recalling that $p \geq 0$ is the dimensionless number that appears in the phase space point (p, c) and R has the dimension [cm], we see that the leading order of (V.116) is *exactly* the classical result and it is independent of the value of $\hbar$ (as expected for the classical order) and of the fiducial lattice spacing μ.
The next-to-leading order correction, on the contrary, has an explicit dependence on μ (since $\eta \propto \mu^2$). It is interesting to observe that in the limit $\mu \to 0$ the correction appears to diverges. However, one is not allowed to draw this conclusion: indeed, for this statement one would have to interchange the limits of t, μ, which is not always allowed. Especially in this case, we approximated the Ashtekar-Lewandowski volume with the Giesel-Thiemann volume, which was derived for $t << \mu$. If this was not the case, it is not to be expected that we can use the replacement from [94]. Indeed, its authors pointed out that the expectation value of $\sqrt{\hat{Q}_v}$ on the coherent states will always stay bounded. Iterating the Cauchy-Schwarz inequality from (II.12) and summing a geometric series: $(n \in \mathbb{N})$

$$\langle \psi, Q_v^{2^{-n}} \psi \rangle = ||\hat{Q}_v^{\frac{1}{2^{n+1}}} \psi|| \leq ||\hat{Q}_v^{\frac{1}{2}} \psi||^{\frac{1}{2}} ||\hat{Q}_v^{2^{-n}} \psi||^{\frac{1}{2}} \leq ... \leq ||\hat{Q}_v^{\frac{1}{2}} \psi||^{1-2^{-n}} = \langle \psi, \hat{Q}_v \psi \rangle^{1-2^{-n}} \tag{V.117}$$

which we find to be finite even for $\mu \to 0$ in (V.111).

However, the corrections at linear order in t for finite values of the parameter μ do have an impact. And it is not clear whether the predictions of these expectation values are in agreement with those of some vectors in a cylindrically consistent Hilbert space, which is just the projection of the continuum theory to resolution $\epsilon = \mu$. Hence, it might be useful to apply the cylindrically consistent renormalisation procedure introduced in chapter *III Renormalisation* by which we hope to obtain the cylindrically consistent Hilbert space, as well as the consistent dynamics on it.
Moreover, it must be mentioned that for general operators these lattice effects will not only be restricted to quantum corrections but might very well have also impact on the classical level. This will present itself in the next subsection, where we shall turn our attention to the Hamiltonian operator and develop an algorithm by which it can be analysed.

V.C.5 An Algorithm for computing Coherent State Expectation Values

We shall now turn our attention to the Hamiltonian operator (and other more general operators). Specifically, we will use the tools presented in the section before to compute the "Cosmological Coherent States Expectation Values" (CCSEV) of the Hamiltonian. In LQC it has been shown that, if one regards this expectation value as the effective Hamiltonian on the (c, p)-phase space, the corresponding effective dynamics agrees with the quantum evolution. Conjecturing that the same might be true for LQG, it is important to evaluate this expectation value in the full theory and compare it with the one obtained in LQC.

The general procedure to obtain an involved expectation value of some operator rests on the following algorithm:

1. Given an operator P which is a polynomial in $\hat{h}, \hat{E}$ and $\hat{Q}$ (possibly involving commutators) on multiple edges $e_{v,i}$ of the lattice (starting at vertex v along direction i). First we create a list L_{cl} of the monomials of P. We search for commutators in P and replace them according to the holonomy-flux algebra (V.21).

2. We will permute the order of the operators for each $P \in L_{cl}$ such that we arrive at the form $\hat{h}...\hat{h}R...R\hat{Q}...\hat{Q}$. For this, we successively replace the order of two elements in $P \in L_{cl}$ by adding their commutator into L_{qu}. We start this procedure with each $\hat{E}^k$, e.g. for string $X = X(h, Q)$

$$..\hat{E}^k(e_{v,i})X... \to X\hat{E}(e_{v,i}) \in L_{cl} \quad \wedge \quad [\hat{E}^k(e_{v,i}), X] \in L_{qu} \tag{V.118}$$

After all $\hat{E}$ appear on the right, we explicitly make a distinction between i being positive, i_+, or being negative, i_-. We can replace these respectively: (see Lemma V.C.3)

$$\hat{E}^k(e_{v,i_+}) \to \mathcal{E} R^k(v, i_+), \qquad \hat{E}^k(e_{v,i_-}) \to \mathcal{E} e^{-izk} R^k(v + e_{i_-}, -i_-) \tag{V.119}$$

where $\mathcal{E} = -i\hbar\kappa\beta/4$.
After this has been done for all $\hat{E}$ we will bring all $\hat{Q}$ to right, by adding once again each commutator into L_{qu} similar to (V.118).
As for the strings in L_{qu} they can be commuted by treating them abelian, as each commutator of them would lead to corrections of order t^2.

3. For $each\ P' \in L_{cl}, L_{qu}$, we create its own new list l, whose generic element $l_{(v,m)}$ (initially equal to 1) can be thought of as a link: one per each combination of $v \in \mathbb{Z}^3_{\mathcal{N}}$ and $m \in \{1,2,3\}$. Moreover, we replace

$$\hat{h}_{ab}(e_{v,i}) \to D_{ab}(v,i), \qquad \hat{h}^\dagger_{ab}(e_{v,i}) \to (-)^{b-a} D_{-b-a}(v+e_i,-i) \tag{V.120}$$

We read P' from right to left and every time we encounter R, D we multiply it on the left of element $l_{(v,m)}$. As this point we have:

$$P' =: c... \prod_{v\in\mathbb{Z}^3} \prod_{m=1..3} l_{(v,m)} Q_v^{N_v} \tag{V.121}$$

where the $c...$ are coefficients whose indices are contracted with the various operators in $l_{(v,m)}$.

4. As each $l_{(v,m)} = D_{a_1b_1}(g)...D_{a_nb_n}(g)R^{k_1}...R^{k_{n'}}$ has an ordering, where n' many R appear on the right, we define its association $\tilde{l}_{(v,m)}$:

$$\tilde{l}_{(v,m)} := \left(\frac{2\eta i}{t}\right)^{n'} \langle D_{a_1b_1}...D_{a_nb_n}\rangle_z \delta_0^{k_1...k_{n'}} \tag{V.122}$$

Afterwards, we replace in both $l_{(v,m)}$ and $\tilde{l}_{(v,m)}$ each appearance of D_{ab} by the following:

$$D_{ab}(g) \to D^{(1/2)}_{aa'}(n_m) D_{a'b'}(g) D^{(1/2)}_{b'b}(n^\dagger_m) \tag{V.123}$$

where $D^{(1/2)}_{aa'}$ is the Wigner-D-function of the $\mathrm{SU}(2)$ element n_m. Since $j = 1/2$ is the defining representation, they equal (V.66).
Finally we collect all links together, for each element $P' \in L_q$:

$$P' = \prod_{v\in\mathbb{Z}^3} \prod_{m=1,2,3} 2^{N_v} \left(\frac{2\eta i}{t}\right)^{N_v} (6i)^{N_v/3} \mathcal{E}^{N_v} \tilde{l}_{(v,m)} =: P_0 \tag{V.124}$$

and for each element $P' \in L_{cl}$:

$$P' = P_0 \left(1 + \sum_{v\in\mathbb{Z}^3} \sum_{m=1,2,3} \frac{1}{\tilde{l}_{(v,m)}} (\langle l_{(v,m)}\rangle_z - \tilde{l}_{(v,m)} + (1 - \delta_{N_v,0}\delta_{N_v+e_m,0}[...]\tilde{l}_{(v,m)})\right) \tag{V.125}$$

$$[...] = (\frac{t}{2^2\eta}(N_v + N_{v+e_m})\partial_\eta + \frac{t}{2^4\eta^2}((N_v + N_{v+e_m})^2 - (N_v + N_{v+e_m})) - \frac{1}{2}(N_v + N_{v+e_m}))$$

where we use explicitly the formulas from the previous section for $\langle l_{(v,m)}\rangle$, i.e. (V.90),(V.106) and those for higher polynomials in D which are still left to be computed.

5. At the end, all elements $P \in L_{cl}, L_{qu}$ have to be contracted with their pre-factors, divided by the normalisation of each link and summed together.

This algorithm can be used to determine, e.g. the expectation value of the scalar constraint. We will only write down the classical contribution of it, which has been computed for the first time in [132]:

$$\langle \hat{C}^\epsilon[1]\rangle = \frac{6V_0}{\kappa}\sqrt{p}\left(\frac{\sin(\mu c)^2}{\mu^2} - \frac{1+\beta^2}{\beta^2}\frac{\sin(2\mu c)^2}{4\mu^2}\right) + \mathcal{O}(t) \tag{V.126}$$

This agrees with the classical expression once we choose the label $\mu = \epsilon$. This could now be considered as an effective Hamiltonian, leading to a resolution of the initial singularity by a Big Bounce as discussed in figure IV.1. However, we want to go even one step further and compare this with other proposals of Big Bounces in the next section.

V.D Loop Quantisation of Symmetry Reduced Models

To stay as close as possible to the model considered above, we will continue to work on the toroidal and compact manifold $\sigma = [0,1)^3$, whose coordinate volume shall be denoted by V_0. We want to emphasise however, that LQC in general is not restricted to this choice, see [284–286].

V.D.1 Classical Symmetries and Regularisation

The philosophy advocated in LQC is the following : From studying the area operator in full LQG, it transpires that it has a discrete spectrum, with smallest non-zero eigenvalue Δ, called the area gap. Now, for constructing the Hamiltonian one considers regularisations which involve the curvature of the connection F^I_{ab}, which is the holonomy of a loop, in other words the boundary of a small surface. It is argued that for its corresponding operator the limit of the loop to zero cannot be taken. The viewpoint that this is not accidental, but a remnant of the intrinsic quantum nature of geometry, leads to the idea that one should not regularise the holonomy adapted to a graph. Instead, it is claimed that there exists an underlying structure, due to which F^I_{ab} is *always* to be regularised in such a way that it attaches a loop, which is the boundary of a surface with area Δ.
If we assume such an underlying structure, it motivates to approximate the classical Hamiltonian in terms of the minimal area loops.

However, this approximation is of course not unambiguous, and one has to carefully detect, which of the many possible quantum predictions due regularisations involving the finite lattice spacing

$$\bar{\mu}^2|p| = \Delta := (2\sqrt{3}\pi\beta)\ell^2_{\rm Pl} \tag{V.127}$$

are the correct one. Indeed, this specific choice has become known in the literature as the $\bar{\mu}$*-scheme* or *improved dynamics*. It can motivated in the following way: Let η be a fiducial metric whose axes of coordinates are along the edges of a cubic lattice. Assuming the lattice is tightly embedded into $\sigma = [0,1)^3$ and each edge carries the function which is the eigenvector to the minimal area eigenvalue Δ. Then the physical area of a slice through σ along two axes of the coordinates can be measured in two different ways, which thus should be equal: $N^2\Delta = |p| = a^2$. On the other hand, the coordinate length ot the torus with respect to the fiducial metric is $1 = N\bar{\mu}$ with $\bar{\mu}$ being the edge length in terms of the fiducial metric. Solving both for N yields (V.127).
It is worth mentioning, that the motivation for the $\bar{\mu}$-choice originated from the fact that the fiducial length scale of the mentioned loops is not computed by an arbitrary kinematic metric of the co-moving coordinates but rather by a physical metric, knowing about the scale factor.

A simplification undergone in LQC is that for flat the Robertson-Walker metric (and only here) we find (see (IV.227))

$$C|_{\cos} = -\frac{1}{\beta^2}C_E|_{\cos} = -\frac{6}{\beta^2\kappa}\sqrt{p}c^2 \tag{V.128}$$

This inspired people to only consider the discretisation of C_E and to promote a term proportional to it to the full scalar constraint operator, which hence can only be valid on the cosmological sector. Indeed, this classical identity works only in the continuum as a discretisation of the general constraint lead us to a natural alternative regularisation (IV.239) where C^ϵ is manifestly *not* proportional to C^ϵ_E. In the following, we will hence compare how these regularisations compare against each other by adapting in both cases the fundamental Δ area gap as discretisation parameter.

While the first case has been excessively studied in [286], the second case was newly treated in [134]. First, we will change the variables on the kinematical level:

$$b := c\bar{\mu}, \qquad V := p^{3/2}, \qquad V = \alpha v =: 2\pi\beta\sqrt{\Delta}G\hbar|v| \tag{V.129}$$

Note that if larger values of p are considered, due to (V.127), the better the approximation $c \approx \sin(b)/\bar{\mu}$ becomes.
Moreover, it implies for the Poisson bracket:

$$\{p,c\} = \frac{\kappa\beta}{6V_0} \Rightarrow \{V,b\} = \sqrt{\Delta}\frac{\kappa\beta}{4V_0} \tag{V.130}$$

$$\Rightarrow \{v,b\} = \frac{\kappa}{V_0 8\pi G\hbar} \tag{V.131}$$

where V_0 is the coordinate volume of the compact torus, we were considering. In the following we will set $V_0 = 1$.
As we discussed above, we will now pick the finite discretisation $\epsilon = \bar{\mu}$ and regularise each loop $\Box^\epsilon$ in C^ϵ_E to be the boundary of a surface with area Δ. The holonomy along an edge e_i in direction i and of length ϵ reads in the classical Robertson-Walker spacetime:

$$h(e_i)|_{\cos} = \exp(sgn(i)c\epsilon\tau_{|i|}) \tag{V.132}$$

and the classical evaluation of the Euclidian part of the scalar constraint has already been carried out in (IV.236):

$$\begin{aligned} C_E^\epsilon|_{\cos}(v) &= \frac{-4}{\kappa^2\beta T_v}\epsilon(i,j,k) tr\left(h(\square^\epsilon_{ij} - h(\square^\epsilon)_{ji})h(e_k)\{h(e_k)^\dagger, V_\epsilon\}\right) = \\ &= \frac{-4}{\kappa^2\beta T_v}\epsilon(i,j,k) 2sgb(ij)\sin(\bar{\mu}c)^2\epsilon_{IJK} tr(\tau_K h(e_k)\{h(e_k)^\dagger, V_\epsilon\}) = \\ &= \sin(b)\left[\frac{-8}{\kappa^2\beta T_v}2^3 tr(\tau_K h(e_K)\{h(e_K)^\dagger, V_\epsilon\})\right]\sin(b) \end{aligned} \tag{V.133}$$

We contract this now with $N(v)$ over all vertices v associated to regions of size ϵ^{-3}. If we would solve the Poisson brackets via symplectic reduction this yielded in total

$$C_E^\epsilon[N]|_{\cos} = \frac{6N}{\kappa\bar{\mu}^2}V^{1/2}\sin(b)^2 \tag{V.134}$$

And doing the same for the full C, i.e. first regulating via ϵ and then evaluating it on cosmology at $\epsilon = \bar{\mu}$ resulted in (IV.239)

$$C^\epsilon\ |_{\cos}\ [N] = \frac{6N}{\kappa\bar{\mu}^2}V^{1/3}\left(\sin(b)^2 - \frac{1+\beta^2}{4\beta^2}\sin(2b)^2\right) \tag{V.135}$$

which we find to be manifestly different from $C_E^\epsilon|_{\cos}$. Thus, we see that if we first regularise and then evaluate on the cosmological level, the starting point of LQC (V.128) is not obtained. This could mean that the philosophy of LQC includes first reducing to cosmology and then regularising. I.e., too consider $(C|_{\cos})^\epsilon$ and afterwards regularise which means sending $b \mapsto \sin(b) + \mathcal{O}(\sqrt{\Delta})$.

V.D.2 Dirac Quantisation in LQC

We will only give a brief overview of how the kinematical Hilbert space is defined. For further details, we refer to [82–84].

It became customary in LQC to work with the so-called "inverse volume corrections". By this is meant that instead of promoting (V.134) straightforwardly to an operator, we keep the regularised version of (V.133). Following this strategy, we will promote this to the scalar constraint operator, as well as its pendant for $C^\epsilon|_{\cos}$. We promote the volume to a multiplication operator on $\mathcal{H}_{LQC} := L_2(\mathbb{R}_{Bohr}, d\mu_{Bohr}(v))$ of square integrable functions on the Bohr compactification of the real line [286, 287] and introduce a shift operator:

$$\hat{V}\psi(v) = V\psi(v) =: \alpha|v|\psi(v), \qquad \hat{N}\psi(v) = \psi(v+1), \qquad \psi \in \mathcal{H}_{LQC} \tag{V.136}$$

By the usual argument on position space, where its canonical conjugated variable becomes a derivative, we find:

$$e^{ik\hat{b}/2}\psi(v) = e^{k\frac{\partial}{\partial v}}\psi(v) = \psi(v+k) \tag{V.137}$$

which allows us to straightforwardly construct the following operator:

$$\sin(\hat{b})\psi(v) := \frac{1}{2i}(\hat{N} - \hat{N}^{-1})\psi(v) \tag{V.138}$$

and similar for $\cos(\hat{b})$. Now using (IV.141), we can build the $\mathrm{SU}(2)$-valued operator for the symmetry reduced holonomy:

$$h(e_k)(\hat{b}) := \cos(\hat{b}/2)\mathbb{1}_2 + 2\sin(\hat{b}/2)\tau_k \tag{V.139}$$

This enables us to evaluate the "inverse volume corrections", for which we find after a short computation:

$$h(e_k)(\hat{b})[h(e_k^{-1})(\hat{b}), \hat{V}]\psi(v) = -\alpha\left[\left(\frac{|v+1| + |v-1|}{2} - |v|\right)\mathbb{1}_2 + i(|v+1| - |v-1|)\tau_k\right]\psi(v) \tag{V.140}$$

With all of the tools at hand, we can finally promote (V.133) in the symmetric ordering it was presented there, to an operator on the Hilbert space of LQC.

After several steps one finds

$$\hat{C}^{\epsilon}_{E}\,|_{\cos}\,[N]\psi(v) := \frac{3\alpha^2 N}{2\kappa^2\beta\hbar\Delta^{3/2}}\left[f(v+2)\hat{N}^4 - (f(v+2)+f(v-2)) + f(v-2)\hat{N}^{-4}\right]\psi(v) \tag{V.141}$$

and for the full scalar constraint

$$\hat{C}^{\epsilon}|_{\cos}[N]\psi(v) = \hat{C}^{\epsilon}_{E}[N] - \frac{3^3\alpha^6(\beta^2+1)N}{2^5\hbar^5\beta^7\kappa^6\Delta^{7/2}}(G(v+4)\hat{N}^8 - G_0(v) + G(v-4)\hat{N}^{-8})\psi(v) \tag{V.142}$$

with

$$f(v) = -|v|B(v), \qquad B(v) = (|v+1| - |v-1|)\,, \qquad G(v) = |v|B(v)g_0(v+2)g_0(v-2), \tag{V.143}$$

$$g_0(v) = (|v+3| - |v-1|)f(v+1) - (|v+1| - |v-3|)f(v-1), \tag{V.144}$$

$$G_0(v) = |v+4|B(V+4)g_0(v+2)^2 + |v-4|B(v-4)g_0(v-2)^2 \tag{V.145}$$

This finishes the Dirac procedure of Quantisation for the symmetry reduced model.

V.D.3 Comparison of Different Regularisations in LQC

We will quickly discuss how the two different operators of the previous subsection can be compared to each other in the context of a coherent state evaluation.

If one considers a Klein-Gordon equation as dust, one could either set $\hat{\Theta}_{LQC} := -\frac{1}{\beta^2}(\hat{V}\hat{C}^{\epsilon}_{E}|_{\cos}[N] + \hat{C}^{\epsilon}_{E}|_{\cos}[N]\hat{V})/2$ to obtain the LQC description, or $\hat{\Theta}' := (\hat{V}\hat{C}^{\epsilon}\,|_{\cos}\,[N] + \hat{C}^{\epsilon}\,|_{\cos}\,[N]\hat{V})/2$ to obtain the newly regularised theory. The dynamics is governed by a Schrödinger evolution equation

$$-i\partial_\phi\Psi(v,\phi) = \sqrt{|\hat{\Theta}_{LQC}|}\Psi(v,\phi) \tag{V.146}$$

(and respectively for $\hat{\Theta}'$). This will be numerically evolved, starting with the states

$$\Psi(v,\phi) = \int_0^\infty dk\;\exp(-(k-k_0)^2/4\sigma^2)e_{k,0}(v)e^{i\sqrt{12\pi G}k\phi} \tag{V.147}$$

which are peaked on $k_0 \in \mathbb{R}$ in Fourier space with spread σ. $e_{k,0}(v)$ is the asymptotic eigenstate of the dynamics as derived in [286] and [134] respectively. The dynamics it produces is presented in figure V.2.

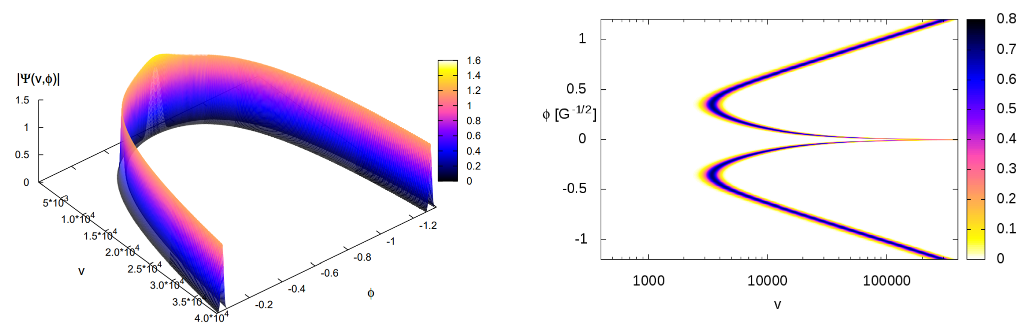

Abbildung V.2: The evolution of a wave packet, explicitly a function over the volume, close to the singularity in different cosmological models of QG. We present $|\Psi(v,\phi)|$, the absolute value of the function over v at different instances of the clock field ϕ differently coloured depending on its numerical value. At late times $\phi \approx 0$ (on the left) and $\phi \approx 1$ (on the right) the function has been chosen to be a coherent state (V.147) and has been evolved *backwards* through the "initial singularity". In the picture on the left (taken from [286]) one sees the standard LQC symmetric Bounce, which is obtained from (V.141), and on the right (taken from [134]) one sees the evolution induced by (V.142). The latter one features an asymmetric Bounce with a past universe dominated by a cosmological constant, which at clock time $\phi = 0$ branches to a symmetric copy of itself.

Let us discuss the choice $\hat{\Theta}'$ in detail: *backwards*, i.e. from bigger to lower ϕ values, we observe:

1. An expanding phase following classical GR
2. Departure from classical dynamics
3. A Bounce resolving the classical singularity
4. Transition to a contracting deSitter phase
5. Transition through $\phi = 0$ (future conformal infinity), where the universe (region) volume reaches infinity
6. Expanding deSitter phase
7. Another Bounce at $-0.35G^{-1/2}$
8. Contraction phase of the dynamics approaching the classical solution in the far past

In fact, the effective Hamiltonian (V.135) coincides with the leading order of the expectation value with striking agreement. It is also interesting to note that there exists a deSitter epoch, i.e. an epoch dominated by a huge cosmological constant. On the one hand, this epoch is future/past complete and hence the sectors for $\phi > 0$ and $\phi < 0$ constitute of separate universes from the classical spacetime perspective. On the other hand, the trajectories of any observable as functions of ϕ have a unique analytic extension through that point. Therefore, from the quantum theory perspective, it might be natural to consider both sections as being parts of the same universe. Independently of which point of view one likes to take, it transpires that it is vastly different than the dynamics in standard LQC where the Bounce is found to be symmetric.

Both models however, differ only in their corrections of order $\bar{\mu}$ (notably in the effective dynamics, the Lorentzian part is $\sim \sin(b)^2$ for standard LQC and $\sim \sin(2b)^2$ for the LQG inspired regularisation). At the moment where the Bounce occurs, b and $\bar{\mu}$ reach their maximal value, and the influence from these corrections becomes dominant. This causes the Bounce, but at the same time implies that its details are highly influenced by the choice of the aforementioned corrections (that is also what our analysis has shown). Hence, some additional arguments are needed telling us which regularisation to favour. To the best of our knowledge a very promising candidate could be a cylindrically consistent regularisation of the Hamiltonian. This motivates our hope that understanding the details of the resolution of the initial singularity can be achieved by applying the framework of direct Hamiltonian renormalisation developed in the third chapter to Loop Quantum Gravity.

Kapitel VI

Conclusion and Outlook

In this chapter, we briefly summarise what the achievements of this thesis have been. Finally, we will comment on directions which further research on this subject could explore.

We have closely investigated the procedure by which a mathematically well-defined quantum field theory can be built. As it transpired, it was pivotal in this construction to choose the correct representation of the algebra of observables out of infinitely many. By studying the projections of the theory at a given resolution, it can be achieved to map the problem of defining a quantum theory of infinitely many degrees of freedom to one of finitely many of degrees of freedom.
However, the observables of the field theory, e.g. the Hamiltonian as the generator of time translation, will not be of a form where they can be written exactly as a function of observables at any finite resolution. Instead, one has to approximate them accordingly and use this approximation to define the corresponding quantum operators. However, the deviation from the continuum theory due to these approximations is now manifestly integrated in the quantum theory and hence affecting the physical predictions of all quantities. Since there are many approximations, we had to find a way to deal with these *quantisation ambiguities*.

In a concrete example, we could find out that these ambiguities indeed change the physical predictions quite drastically: General Relativity presents a field theory describing the geometry of our universe. Its predictions were hugely successful, e.g. isotropic models simulating the behaviour of our universe on large scales like the Robertson-Walker metric. Its quantum theory, however, remains unknown as of today. Yet, its necessity is obvious because of the breakdown of General Relativity, for example in the *Big Bang* singularity predicted by the Robertson-Walker metric.
We studied a concrete discretisation of General Relativity and found that at a fixed resolution an approximation to the dynamics would *on the classical level* resolve the Big Bang singularity by replacing it with a Big Bounce, implying that prior to ours there was an old contracting universe. This Big Bounce remains in the theory during the process of canonical quantisation where, at some point, an ad-hoc regularisation of the scalar constraint had to be chosen. Further analysis showed that, in models of canonical Quantum Gravity, the choice of the discretisation has non-trivial impact on the details of the singularity resolution. Due to the mathematical precise language of the earlier works in LQG, we are able to investigate and confirm this again by computing the expectation value of the scalar constraint with respect to coherent states. It leads us to believe that one has to be careful with the details of the resolution of the Big Bang until these quantisation ambiguities have been fixed.

In this thesis, we have now been extending already existing methods to resolve the ambiguities, i.e. we introduced a Hamiltonian version of the *renormalisation group*. As renormalisation was originally created in the path integral approach towards quantisation, the first task was to compare the latter with canonical quantisation. We generalised ideas from the literature to present not only a way to obtain a Hamiltonian formalism from a history space measure (which is known as Osterwalder-Schrader reconstruction), but moreover demonstrated that for each Hamiltonian theory obtained in this way, we can construct a corresponding history space measure.
Due to this bijection, we were now able to develop a renormalisation procedure which remains completely in the Hamiltonian framework and produces the same fixed point theory as the path integral renormalisation. However, this Hamiltonian scheme came with a caveat: namely, it forced us to compute the renormalisation of the path integral measure simultaneously. As it was originally our goal to circumvent the latter construction, we altered the path-integral induced Hamiltonian renormalisation minimally. The *direct Hamiltonian renormalisation* was designed to stay as close as possible to the scheme dictated by the path-integral indu-

ced Hamiltonian renormalisation flow and yield as fixed point still a cylindrically consistent theory. These are quantum theories which are defined on coarse resolution but still capture the correct physical predictions of an underlying continuum quantum theory.
Subsequently, we examined this procedure in the case of the "massive free scalar field". This being a simple non-interacting theory, we had full control over the continuum quantum field theory whose cylindrical projections we wanted to obtain by renormalisation. We managed to find the exact analytic structure of the fixed point in arbitrary dimensions. It is important to note that the fixed point of the path-integral induced Hamiltonian renormalisation and the fixed point of the direct Hamiltonian renormalisation agree in their continuum limit with each other and with the correct continuum quantum theory. This test case shows that at least in some models the direct Hamiltonian renormalisation yields correct results. As it is considerably easier to handle than its counterpart, we should perform more test on it, in order to use it eventually for the renormalisation of Quantum Gravity.
Moreover, in the aforementioned example of the massive free scalar field, we were able to investigate further properties of the direct Hamiltonian renormalisation. As its main goal is to eliminate the ambiguities that arise due to the discretisation, we checked whether different initial discretisations lead to the same fixed point and found the answer to be affirmative. A naive discretisation which approximates the Laplacian by only taking next neighbour differences on the lattice into account was flowing into the same fixed point as a more sophisticated discretisation that considered multiple next-to-next neighbour interactions. This indicates that we maybe do not need to worry which regularisation to pick when trying to find a cylindrically consistent theory of more involved systems.
Moreover, the choice of the coarse-graining map, which defined the flow, has not been unique and indeed different proposals are sufficient for cylindrical consistency. But the fixed point turned out to be even more robust, as it does not matter in the renormalisation prescription what the details of the blockspin-transformation look like. In other words, the renormalisation flow yielded a unique result, independent of the geometric details of the cuboid that is coarse grained. We take from this the hope that any cylindrically consistent map can be used for determining the fixed points of more involved theories such as General Relativity.
The fixed point theory we obtain includes a discretised version of the Laplace operator. Due to the fact that it captures the most important properties of its continuum pendant, it is customary to call it *perfect Laplacian*. We computed its exact analytic form and found that its matrix elements show an exponential drop-off behaviour the further two points on the lattice are separated from each other. Hence, it presents a form of locality which gets increasingly better the finer the resolution of the system becomes.
Finally, we were able to demonstrate for the free field how symmetries of the continuum are restored on the lattice, most notably rotational invariance. While being a property which cannot be exactly implemented on a cubic lattice, we found that one can nonetheless translate it into a non-trivial condition for the fixed point theory. By numerical investigation, it transpired that the free massive scalar field satisfies this condition at fine resolution to a high precision. This indicates that rotational invariance will be recovered in the continuum.

Due to all these considerations we could assure ourselves that the direct Hamiltonian renormalisation is a promising candidate for fixing the quantisation ambiguities which arise during the regularisation process of field theories. For General Relativity, upon introducing suitable reference frames the scalar constraint becomes a physical Hamiltonian and the system fulfils the necessary subset of the Osterwalder-Schrader axioms (i.e. without Euclidean invariance) needed for the methods discussed in this thesis. In this sense the procedure can be applied to canonical Quantum Gravity and one can hope to obtain a cylindrically consistent formulation. This leads us to the considerations for further research.

Further tests of the direct Hamiltonian renormalisation: As the above tests have yielded positive results, we can in principle use the framework directly for Quantum Gravity. On the other hand, one might want to be cautious and verify the Hamiltonian renormalisation flow for other simple systems where at least partial knowledge of the continuum theory is at hand. A promising example for this is the lower dimensional interacting $P(\phi)_2$ QFT [296].
Another example is a compactified scalar field $\phi \to \sin(\phi\epsilon)/\epsilon$ in the free field Lagrangian. This would present a good test to see what happens once compact fields enter the picture which is unavoidable in the context of gauge theories, to which GR in its Ashtekar formulation belongs.

Extension of the Hamiltonian renormalisation to (non-abelian) gauge theories: When quantising Yang-Mills theories, one is naturally lead to the framework of holonomies, which are defined along curves. This is in contrast to the scalar fields smeared over 3-dimensional regions and hence implies that the definition

of the injection maps $I_{M\to 2M}$, which give rise to cylindrical consistency, must be considerably different.
The first to check would be free Maxwell QFT, which is a gauge theory over the abelian group $\mathrm{U}(1)$ and, moreover, still a free theory. Hence, we again have control over the continuum QFT and can compare the results of the renormalisation procedure. The next step would then be the extension to non-abelian gauge groups, most notably $\mathrm{SU}(2)$ and $\mathrm{SU}(3)$, which describe weak and strong interaction respectively. This is also a crucial prerequisite for studying GR as the Ashtekar connection is $\mathfrak{su}(2)$-valued.

Renormalisation of the $\mathrm{U}(1)^3$ approximation of Loop Quantum Gravity: Although LQG is the quantisation of an $\mathrm{SU}(2)$ gauge theory, one could classically rewrite it using abelian holonomies. Albeit spoiling the nice transformation properties of the holonomies under gauge transformations, this motivates to consider an alternative quantisation using the group $\mathrm{U}(1)^3$. As shown in [93], this yielded indeed the correct semi-classical limit of GR on a lattice.
Hence, a first step towards studying the properties of the renormalisation flow in LQG would be to use this approximation, as the renormalisation of an abelian theory is considerably easier than of a non-abelian one. Although it will not be the final answer, one could hope to gain useful insights for the general case when studying the fixed points obtained in this case.

Renormalisation of full Loop Quantum Gravity: Once the aforementioned steps have been completed, one will hopefully have found a good candidate for the initial discretisation in LQG. Then, we can use it to start the direct Hamiltonian renormalisation. It will be interesting to investigate how the volume transforms under a renormalisation step and whether the Ashtekar-Lewandowski vacuum might not be annihilated by all elements in the sequence $(\hat{C}^{\epsilon})^{(n)}$. Should this happen, it might suggest that some of the regularity properties of the uniqueness theorem [68] had been too strong to be demanded.
Finally, we must determine the cylindrically consistent fixed point family $(\mathcal{H}^*_M, \hat{C}^*_M, \Omega^*_M)$ of Loop Quantum Gravity in order to make physical predictions.

Stable coherent states in Loop Quantum Gravity: The toolbox to obtain an effective Hamiltonian from the initial discretised quantum gravity theory used coherent states peaked on a Robertson-Walker spacetime. However, it is not clear whether these states will remain sharply peaked under time evolution. If the quantum effects blow up, the terminus "effective Hamiltonian" would have been assigned prematurely.
The solution must be to find coherent states which remain stable under time evolution and use them in order to compute the effective Hamiltonian. A possible strategy to tackle this problem might be to use the concept of Fourier Integral Operators [297–299].

Cosmological Coherent State Expectation Values in cylindrically consistent LQG: After having achieved the fixed point theory of canonical QG, it must be put to the test and used to extract physics from it. As the toolbox of the cosmological coherent state expectation values has proven successful for the initial discretisation, it will hopefully translate to coherent states in the cylindrically consistent Hilbert space and be applicable for the Hamiltonian obtained by deparametrisation from the fixed point scalar constraint. Ideally, this happens after one has constructed the stable coherent states of cosmology.

Determine the cosmological subsector of LQG: While being a good starting point, the cosmological coherent states are by no means perfect candidates for an LQG solution for continuum cosmology. One could look at them as cylindrical projections of a yet unknown cosmology solution in the continuum Hilbert space. Ultimately, one would like to find these states. First proposals in this direction have already been undergone in [300, 301], by introducing an "isotropy constraint" operator. The proposal in the literature, however, lacks the same known regularisation ambiguities and must be suitably altered if its cylindrical projections fail to annihilate the cosmological coherent states.

Extending the toolbox of the Cosmological Coherent States Expectation Values: There are still crucial building blocks missing in order to compute the expectation values of *every* operator defined on the kinematical Hilbert space of LQG. As the renormalised Hamiltonian might be of a type which is not covered yet, this toolbox must be completed in time. It will then also include the possibility to compute the expectation values of higher time derivatives of geometric operators.
As these tasks tend to become more and more involved with the increasingly hard combinatorial structure of the operators, a natural extension would be to build a numerical code which is able to execute the calculations that are part of the algorithm presented in this thesis.

Coherent States for different symmetric spacetimes: In this thesis, we only considered the flat

Robertson-Walker metric, but it is (at least conceptually) straightforwardly extendible to other semi-classical models. Among the most interesting ones are probably Robertson-Walker spacetimes with non-vanishing curvature, as well as spherically symmetric situations, e.g. black holes.
Moreover, one should finally include the Standard Model and study the Yang-Mills degrees of freedom on semi-classical spacetimes which could be viewed as an improvement of [302].
Next to different spacetimes, we might also consider different choices of the graph for each spacetime, e.g. cubical or spherical lattices. For a cylindrically consistent projection, the details will look different in each case, albeit the physical predictions should not change. However, as of today this is unconfirmed.

Implementing a cylindrically consistent version of Loop Quantum Cosmology: We had discussed, in the main text, that even LQC is prone to the quantisation ambiguities that occur due to the choice of a regularisation. Moreover, each ambiguity can be related to some choice in full canonical QG. Hence, once the choices leading to the renormalised fixed point in full LQG are known, we can use them to construct a consistent Hamiltonian for Quantum Cosmology, hopefully presenting a reliable quantum resolution of the initial singularity.

Abbildungsverzeichnis

Notations and conventions

$(\mathcal{M}, g_{\mu\nu})$	Riemannian spacetime consisting of a manifold and a metric tensor, $(-+++)$
$C(\mathcal{M})$	space of all continous functions from $\mathcal{M}$ to $\mathbb{C}$
$\mathcal{S}(\mathcal{M})$	Schwartz fns. of rapid decrease, i.e. going to zero faster than any polynomial
(σ, q_{ab})	spatial hypersurface, embedded into $\mathcal{M}$ and equipped with a spatial metric
$\mathrm{Diff}(\mathcal{M})$	group of all smooth diffeomorphisms on $\mathcal{M}$
$\mathcal{L}_v$	Lie derivative with respect to vector field v^a
∇	metric-compatible Levi-Civita connection with Christoffel symbols $\Gamma^\rho_{\mu\nu}$
$R^\sigma_{\mu\nu\rho}, R$	Riemann curvature tensor and Ricci scalar
κ	Gravitational coupling constant $(16\pi G c^{-4})$
N, N^a	lapse and shift function
K_{ab}	extrinsic curvature
$C,\ C_a$	scalar or Hamiltonian constraint and (spatial) diffeomorphism constraint
A^I_a, E^a_I	$\mathrm{SU}(2)$ connection and electric field, $a = 1,2,3$, $I = 1,2,3$
β	Immirzi parameter
$V(R)$	Volume of region R
F^I_{ab}	curvature as a function of the connection A
G_J	$\mathrm{SU}(2)$-Gauss constraint
τ_I	basis of $\mathfrak{su}(2)$, $(I = 1,2,3)$ with $\tau_I := -i\sigma_I/2$ and σ_I being the Pauli matrices
α^Λ_s	Hamiltonian flow of certain gauge transformation smeared with Λ
$h(e)$	holonomy along a path e of an associated $\mathrm{SU}(2)$ connection
$E_f(S)$	electric flux through a surface S contracted with f^J.
$g_k,\ a(t)$	Robertson-Walker metric with curvature k and with scale factor $a(t)$
(c, p)	symplectic reduction of (A^I_a, E^J_b) for an isotropic spacetime
$\mathcal{H}$	Hilbert space endowed with a sesquilinear, positive definite scalar product $\langle .,. \rangle$
$\mathcal{L}(\mathcal{H})/\mathcal{B}(\mathcal{H})$	space of all/bounded operators on $\mathcal{H}$
μ_G	left- and right-invariant Haar measure of a compact Lie group G
$(\pi^{(j)}, \mathcal{H}^{(j)})$	irreducible representation of a unital algebra $\mathcal{A}$
$(\Pi^{(j)}, \mathcal{H}^{(j)})$	irreducible representation of a Lie group G
$\mathcal{A}, \omega$	$*$-Lie-algebra of observables with the positive functional ω, called state
$(\pi, \mathcal{H}, \Omega)$	GNS triple with cyclic vector Ω (in 1:1 correspondence with state ω)
W_n	Wightman n-point functions, defined in Minkowski space $\{(t_i, \bar{x}_i)\}_{i=1\ldots n}$
S_n	Schwinger n-point functions, defined in Euclidian space as $\mathrm{W}_n \mid_{t_i \to i\beta_i}$
E_n	Euclidian n-point functions, obtained from the generating functional $S[F]$
$\hat{H}, \hat{\phi}$	Hamiltonian- and canonical field-operators on $\mathcal{H}$
$U(t)$	operator of finite time translation t, generated by $\hat{H}$ with $U(t) = \exp(-it\hat{H})$
$R,\ T$	spatial and temporal infrared (IR) cut-offs
$\epsilon,\ \delta$	spatial and temporal ultraviolet (UV) cut-offs
μ_M	family of discretised path integral measures at resolution M
$(\mathcal{H}_M, \hat{H}_M, \Omega_M)$	family of discretised OS data
I_M, E_M	Injection and evaluation map of resolution M (with suppressed label R)
$I_{M\to 2M}$	cylindrically consistent coarse graining map
$L_{T,R}$	space of L_2 functions on the compactified manifold $[0,T) \times [0,R)^D$
$L_{N,M}$	space $l_2(\mathbb{Z}_N, \mathbb{Z}^D_M)$ with scalar product $\langle .,. \rangle_{N,M}$
ω_{AL}	unique, diffeomorphism invariant Ashtekar-Isham Lewandowski state
$\hat{V}_{AL}(B), \hat{Ar}(S)$	Ashtekar-Lewandowski volume operator and area operator
$\psi^t_{e,h^{\mathbb{C}}_e}$	Complexifier coherent state peaked at $h^{\mathbb{C}}_e \in SL(2,\mathbb{C})$ with spread t
$\Psi_{(c,p)}$	cosmological coherent state on graph γ of a (c,p)-Robertson-Walker metric
$R_\tau,\ L_\tau$	Right- and left-invariant vector field in direction τ
$D^{(j)}_{mn}(g)$	Wigner-D-matrix function of group element $g \in \mathrm{SU}(2)$
$\bar{\mu} = \sqrt{\Delta/\lvert p \rvert}$	dynamical regularisation parameter of LQC, with area gap $\Delta = (2\sqrt{3}\pi\beta)\ell^2_{\mathrm{Pl}}$

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I hereby assure that I've written this thesis on my own while using nothing but the quoted resources.

Erlangen, date	Klaus Liegener