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LOOP QUANTUM COSMOLOGY:
ANISOTROPIES AND INHOMOGENEITIES

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Abstract

In this dissertation we extend the improved dynamics of loop quantum cosmology from the homogeneous and isotropic Friedmann-Lemaître-Robertson-Walker space-times to cosmological models which allow anisotropies and inhomogeneities. Specifically, we consider the cases of the homogeneous but anisotropic Bianchi type I, II and IX models with a massless scalar field as well as the vacuum, inhomogeneous, linearly polarized Gowdy T^3 model. For each case, we derive the Hamiltonian constraint operator and study its properties. In particular, we show how in all of these models the classical big bang and big crunch singularities are resolved due to quantum gravity effects. Since the Bianchi models play a key role in the Belinskii, Khalatnikov and Lifshitz conjecture regarding the nature of generic space-like singularities in general relativity, the quantum dynamics of the Bianchi cosmologies are likely to provide considerable intuition about the fate of such singularities in quantum gravity. In addition, the results obtained here provide an important step toward the full loop quantization of cosmological space-times that allow generic inhomogeneities; this would provide falsifiable predictions that could be compared to observations.

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For my family

Chapter 1

Introduction

1.1 Quantum Gravity

The two theories of quantum mechanics and general relativity revolutionized the field of physics in the twentieth century; both of these theories have been remarkably successful and have greatly enhanced our understanding of the natural world. While quantum mechanics describes the small scale behaviour of elementary particles, atoms and molecules, general relativity is the classical theory of gravity used to describe large systems such as the solar system, galaxies or even the universe as a whole. By and large, quantum effects are not relevant in the study of the macroscopic systems described by general relativity, and since gravity is such a weak force, it can safely be ignored in the small-scale regimes where quantum effects are important. Due to this split, only one or the other of these theories is necessary to describe the vast majority of physical phenomena since the effects due to the other will be negligible.

However, in some cases it is expected that quantum effects and gravity will simultaneously be important, especially when a large mass is confined in a small region as happens, for example, in the cases of black holes and the very early universe when the matter energy density was extremely high. In order to accurately describe the physics of these systems, one must develop a theory which combines the two: a theory of quantum gravity.

To date, it has been extremely difficult to construct such a theory. There are currently several candidate theories including asymptotic safety, causal dynamical triangulations, causal sets, noncommutative geometry, string theory, supergravity and the focus of this dissertation, loop quantum gravity. At this point, it is important to note that all of these theories are currently incomplete and that none of them have yet offered any falsifiable predictions. Nonetheless, recent progress in many of these diverse approaches has been encouraging; in particular, there have recently been some interesting results in the field of loop quantum gravity. For an introduction to loop quantum gravity, see, e.g., [1, 2, 3].

Loop quantum gravity (LQG) is a background independent, nonperturbative approach to quantum gravity where the space-time geometry is treated quantum mechanically from the very beginning. One starts from a classical theory of gravity where the elementary variables are an $SU(2)$-valued connection A_a^i and its conjugate momentum, the densitized triad E_i^a (i.e., triads with density weight one) [4, 5, 6, 7]. This is a particularly appealing choice of variables as they are very similar to the variables used in Yang-Mills theories where the quantum theory is well understood. However, the theory here is more complicated due to the presence of the Hamiltonian and diffeomorphism constraints in addition to the Gauss constraint: major complications arise as gauge symmetries now include space-time transformations and hence dynamics. Nonetheless, the similarities between the two theories are helpful. Taking holonomies of the connection and fluxes of the densitized triads as the elementary operators in the quantum theory, one obtains the Ashtekar-Isham algebra [8] providing the point of departure for quantum theory. A very surprising result due to Lewandowski, Okolow, Sahlmann, Thiemann and Fleischhack [9, 10] is that, modulo certain technical conditions which implement physical ideas precisely, the algebra admits a unique (cyclic) representation in which the diffeomorphism group is unitarily implemented. Thus, thanks to the underlying diffeomorphism invariance, there is a unique kinematical arena in quantum gravity. Even more surprising is the fact that in this representation, the spectrum of geometrical operators such as area and volume is discrete [11, 12]. The next step that remains to be taken is to obtain the physical Hilbert space. In order to do this, one must construct the Hamiltonian constraint operator and it is not yet fully understood how to do this in full generality. However, in the last few years there has been some work showing how the Hamiltonian constraint operator can be built if there is a matter field —such as dust or a scalar field— available that can be used as a clock and a measuring rod [13, 14].

There have also been some recent developments in spin foam models [15] —an approach to quantum gravity which is hoped to be the covariant form of LQG— regarding the form of the vertex amplitude [16] which give some strong indications that spin foams and LQG may indeed be related; only a few years ago this had not yet been very clear. Some other results in LQG include the calculation of the entropy of a black hole which gives the semi-classical result of a quarter of the black hole's surface area in Planck units plus a logarithmic correction [17, 18], and a reduced phase space quantization of some simple cosmological models in what is called loop quantum cosmology where one can see that the classical big bang and big crunch singularities are resolved due to quantum geometry effects.

1.2 Loop Quantum Cosmology

Thanks to spectacular advances in observational cosmology, the early universe now offers an ideal ground for confronting quantum gravity theories with observations. It is therefore of great interest to apply basic ideas of loop quantum gravity to cosmology. However, as pointed out in the previous section, it is not yet fully understood how to implement the dynamics of LQG in full generality. Luckily, observations indicate that our universe is approximately homogeneous and isotropic at large scales. These symmetries allow a mathematical description of the large-scale structure of our universe to be much simpler than it would have been otherwise.

In loop quantum cosmology, one studies the quantization of symmetric space-times following the ideas and methods of loop quantum gravity. Due to their high degree of symmetry, the space-times can often be described by a finite number of degrees of freedom (a minisuperspace) and then quantum mechanics, rather than quantum field theory, is sufficient to describe the quantum theory. Because of this simplicity, many of the technical complications of full loop quantum gravity go away and it is possible to make further, concrete progress. Since one wants to follow LQG, the operators in LQC are also fluxes of the densitized triads (i.e., areas of surfaces) and holonomies of the connection. However, due to the high symmetry of the models, it is no longer necessary to consider all surfaces and all paths: a few carefully chosen surfaces and paths will suffice. Clearly, this greatly simplifies the quantization procedure as compared with the full theory. Reviews of LQC are given in, e.g., [19, 20, 21, 22, 23].

When I began my dissertation, much of the work in LQC thus far had concentrated on the relatively simple case of the homogeneous and isotropic Friedmann-Lemaître-Robertson-Walker (FLRW) cosmological models, often with a massless scalar field which plays the role of a relational clock. For example, the theory concerning the flat FLRW model was progressively developed in [24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42]. In the FLRW models, quantum geometry effects due to LQG have been shown to create a new repulsive force in the Planck regime. The force is so strong that the big bang is replaced by a specific type of quantum bounce: the force rises very quickly once the scalar curvature reaches $\sim -0.15\pi/\ell_{\rm Pl}^2$ (or once the matter energy density ρ reaches $\sim 0.01\,\rho_{\rm Pl}$) to cause the bounce, but it also dies very quickly after the bounce once the scalar curvature and the density fall below these values. Therefore, outside the Planck regime, the quantum space-time of LQC is very well approximated by the space-time continuum of general relativity. This scenario is borne out in the k=0, Λ=0 models [34, 35], $\Lambda \neq$0 models [43, 44, 45], the k=+1 closed model [46, 47], k=-1 open model [48, 49] and the k=0 model with an inflationary potential with phenomenologically viable parameters [50]. Note that the space-time is extended as it is no longer truncated by a big bang or a big crunch singularity as in the classical theory. Going beyond the big bang and big crunch singularities, LQC has also been used to argue that its quantum geometry effects resolve all strong curvature singularities in homogeneous, isotropic situations in which the matter field is a perfect fluid with an equation of state of the standard type, $p = p(\rho)$ [51].

As mentioned above, one of the key features in LQC is that the curvature is expressed in terms of holonomies and one must determine how these holonomies are to be constructed. In particular, the length ℓ of the holonomies must be fixed in some manner. In the earlier LQC papers, ℓ was taken to be a constant (the so-called μ_o scheme) until several difficulties were discovered: in particular, it was shown that it is inconsistent with the current inflationary paradigm [52, 53] and also that quantum gravity effects could become significant at arbitrarily low curvatures [33, 34]. A more careful analysis [34] showed that, in order to obtain the correct semi-classical limit, one should rather use the $\bar{\mu}$ scheme (also called the "improved dynamics") where ℓ depends on the state that is being acted upon by the holonomy. At a mathematical level, it is more difficult to study a theory where ℓ depends on the wave function rather than simply being constant, but it turns out that the resulting physics is much better behaved: the $\bar{\mu}$ formulation of LQC is compatible with inflation and quantum gravity effects only become important when the curvature reaches the Planck scale, just as one would expect.

In order to understand the dynamics of the very early universe, one must consider quantum gravity phenomena. Although a full derivation of LQC from LQG has not yet been achieved, LQC is expected to correctly capture at least the qualitative behaviour of the full theory for those degrees of freedom which are responsible for the most important features of our universe. Because of this, there has already been some preliminary work considering possible imprints in the spectra of the cosmic microwave background and primordial gravitational waves due to LQC [54, 55, 56]. These works are necessarily incomplete as it is not yet understood how generic inhomogeneities can be properly incorporated in LQC, but they provide important first steps toward the ultimate goal of deriving a falsifiable prediction for LQC in the future.

In addition, there has been a remarkable confluence between LQC and several other fields. For example, the holographic principle, as embodied by the covariant entropy bound, has been shown to hold in LQC in situations where it fails classically[1] [57]. In general relativity, as one approaches the big bang, physical quantities such as the space-time curvature, the matter energy density, the temperature and the entropy density diverge. Due to the divergence of the entropy density, the covariant entropy bound fails in a region very close to the big bang. In LQC, the singularity is resolved by quantum gravity effects and therefore physical quantities no longer diverge; however, they still do become very large and one must check that they do not become so large that the covariant entropy bound is violated, this is verified in [57]. Thus, quantum gravity effects due to LQC save the holographic principle in this setting. LQC seems to provide an ideal arena for slow roll inflation as well: assuming the presence of an inflaton field, the likelihood of obtaining viable initial conditions for slow roll inflation after the quantum bounce

[1] This is research that I did during my graduate work, but it will not form a part of my dissertation.

is higher than 99% [58]. This is a welcome contrast to the classical theory where it has been argued that the *a priori* probability of slow roll inflation is exponentially suppressed [59].

More recently, LQC has been reformulated in a path integral expansion [60, 61, 62, 63, 64] which has a form that is very similar to that of spin foam models, thus providing a link between canonical LQG and covariant spin foam models via the bridge of LQC. These investigations have shed considerable light on some conceptual issues: they have realized the hope that vertex expansions can provide a convergent series for the physical inner product and they have clarified some aspects of the relation between between spin foam models and group field theories (see, e.g., [65] for an introduction to group field theories). On the other hand, it has also raised issues about which quantum geometries one should sum over; in particular, a consistent time orientation appears to be necessary. There is also progress going in the other direction: in spin foam cosmology, one starts from a simple dipole model which captures some of the relevant degrees of freedom (homogeneity and some perturbations thereon) and then studies the resulting physics [66, 67, 68, 69]. The field of spin foam cosmology is still young, but it is already providing some important results: first of all, it allows inhomogeneities from the start, and it also provides a potential avenue to derive LQC from spin foam models.

The development of LQC has also been extremely valuable due to the insights it has provided as a simplified model for the full theory of LQG. First of all, one can address the problem of time by using a matter field as a clock (in most cases a massless scalar field) [32, 33, 34], or one can consider relational observables in more complicated cosmological models where more than one gravitational degree of freedom is available [70]. It also offers some insight into the problem of dynamics: one of the main problems in LQG is to construct the Hamiltonian constraint operator, and since there are many ambiguities in this construction, it is necessary to determine which choices are physically viable and which are not. This is somewhat similar to the possibility of using either the μ_o or $\bar{\mu}$ schemes in LQC where it turns out that the scheme which allows the correct semi-classical limit is $\bar{\mu}$. Although the ambiguities in the full theory are more complicated than what one deals with in LQC, it is hoped that some of these lessons from LQC will be useful and will help to resolve at least some of the ambiguities in the construction of the

Hamiltonian constraint operator. In addition, as mentioned above, it provides a bridge between LQG and spin foam models thus providing more evidence that, as is hoped, the two theories are indeed related.

Now, both in order to test the robustness of LQC and to move toward a more realistic model of our universe, it is important to drop the symmetry requirements that have been imposed in the simpler homogeneous and isotropic models. A first step in this direction is to retain homogeneity and extend LQC to anisotropic situations. In the isotropic case, there is only one nontrivial curvature invariant, the (space-time) scalar curvature (or, equivalently, the matter energy density). In anisotropic situations, Weyl curvature is nonzero and it too diverges at the big bang. Therefore, one can now enter the Planck regime in several inequivalent ways and this suggests that the Planck scale physics will be much richer. A next step would be to allow inhomogeneities in addition to anisotropies, starting in a controlled fashion so that one is not immediately overwhelmed before gradually moving on to allow generic inhomogeneities.

The first step of allowing anisotropies (but still demanding homogeneity) corresponds to the study of the loop quantum cosmology of Bianchi models, while the second step, allowing inhomogeneities in a controlled manner, can be done via the Gowdy model where inhomogeneous modes are only allowed along one of the three spatial directions.

Another motivation to study the Bianchi models in LQC is provided by the Belinski, Khalatnikov and Lifshitz (BKL) conjecture which claims that, as a generic space-like singularity is approached, neighbouring points decouple from one another and the dynamics at each point can be well approximated by the ordinary differential equations of the Bianchi models [71, 72]. If this conjecture is correct, understanding the behaviour of Bianchi models in quantum gravity may be sufficient in order to fully comprehend the fate of general space-like singularities in quantum gravity and the quantum physics in the associated Planck regime.

Of course, the importance of studying the Bianchi and Gowdy models in the context of LQC has been recognized for some time now, and there already exists some pioneering work in this direction. However, much of the early work studying anisotropic models [73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83] was done before isotropic models were completely understood in LQC and in particular before the

$\bar{\mu}$ scheme was introduced. Similarly, the early work studying the Gowdy model in LQC [84, 85] occurred before the improved dynamics of anisotropic models were fully understood and these works used an incorrect generalization of $\bar{\mu}$ for anisotropic models.

The goal of my dissertation is to revisit these models in light of the most recent understandings and to study the improved dynamics loop quantization of Bianchi models and of the simplest Gowdy model, the linearly polarized Gowdy model on T^3.

1.3 Organization

The dissertation is organized as follows: in Chapter 2, the loop quantization of the Bianchi type I model will be examined, based on the work in the paper [86]. Since Bianchi I space-times are spatially flat, they are the simplest case and therefore a good starting point. In Chapters 3 and 4, we will consider the Bianchi type II and type IX models which both allow spatial curvature and whose space-times, in turn, are more complex. These chapters are based on the papers [87] and [88], respectively. Finally, Chapter 5 will concern the hybrid loop/Fock quantization of the linearly polarized Gowdy T^3 model based on the paper [89]; note that its companion paper [90] does not constitute a part of this dissertation. Finally, there are two appendices: the first details the parity symmetries of homogeneous models in LQC while the second compares two possible loop quantizations of the closed FLRW model. At certain points in the dissertation some definitions and results from previous chapters will be repeated so that each chapter is self-contained.

The research I have carried out during my graduate studies has not been limited to the work presented in this dissertation. First, as mentioned above, I have shown how the covariant entropy bound is saved by quantum gravity effects in the context of LQC [57]. I have also worked on the path integral formulation of LQC, in particular deriving a local vertex expansion for the vacuum Bianchi I model [64]. Locality is a key ingredient in spin foam models which was lacking in the earlier LQC vertex expansions and the link between spin foams and the LQC vertex expansions is now much clearer. Finally, I have studied, at a classical level, the surface terms that appear in the action used for loop quantum gravity [91]. This work may allow a direct quantization of boundaries, such as the isolated horizons of black holes, in loop quantum gravity.

Chapter 2

Bianchi Type I Models

2.1 Introduction

Although Bianchi I space-times are the simplest anisotropic cosmological models, results obtained in the context of the BKL conjecture [71, 72] suggest that they are perhaps some of the most interesting ones for the issue of singularity resolution. The BKL conjecture states that, as one approaches space-like singularities in general relativity, terms with time derivatives would dominate over those with spatial derivatives implying that the asymptotic dynamics at each point would be well described by the dynamics of one of the homogeneous Bianchi models, i.e., by an ordinary differential equation. By now considerable evidence has accumulated in favour of this conjecture [92, 93, 94, 95, 96, 97]. For the particular case when the matter source is a massless scalar field (without any symmetry assumptions), these results suggest that as the system enters the Planck regime, dynamics along any fixed spatial point would be well described by a Bianchi I metric. Therefore, understanding the fate of Bianchi I models in LQC could provide substantial intuition for what happens to generic space-like singularities in LQG [98, 99].

Indeed, in cosmological contexts where one has approximate homogeneity, a natural strategy in full LQG is to divide the spatial 3-manifold into small, elementary cells and assume that there is homogeneity in each cell, with fields changing slowly as one moves from one cell to the next. (For an exploration along these lines in the older μ_o scheme, see [100].) Now, if one were to assume that geometry in each elementary cell is also isotropic, then the Weyl tensor in each cell —and therefore everywhere— would be forced to be zero. A natural strategy to accommodate realistic, nonvanishing Weyl curvature would be to use Bianchi I geometry in each cell and let the Bianchi I parameters vary slowly from one cell to another. In this manner, the loop quantum cosmology of the Bianchi I model can pave the way to the analysis of the fate of generic space-like singularities of general relativity in full LQG.

Because of these potential applications, Bianchi I models have already drawn considerable attention in LQC (see in particular [73, 78, 79, 80, 81, 82, 83]). During these investigations, groundwork was laid down which we will use extensively. However, in the spatially noncompact context (i.e., when the spatial topology is $\mathbb{R}^3$ rather than $\mathbb{T}^3$), the construction of the quantum Hamiltonian constraint turned out to be problematic. The Hamiltonian constraint used in the early work has the same difficulties as those encountered in the μ_o scheme in the isotropic case (see, e.g., [39], or Appendix B of [21]). More recent papers have tried to overcome these limitations by mimicking the $\bar{\mu}$ scheme used successfully in the isotropic case. However, to make concrete progress, at a key point in the analysis a simplifying assumption was made without a systematic justification.[1] Unfortunately, it leads to quantum dynamics which depend, even to leading order, on the choice of an auxiliary structure (i.e., the fiducial cell) used in the construction of the Hamiltonian framework [83]. This is a major conceptual drawback. Also, the final results inherit certain features that are not physically viable (e.g., the dependence of the quantum bounce on "directional densities" [79, 80, 81]). We will provide a systematic treatment of quantum dynamics that is free from these drawbacks. As in the isotropic case we will use a massless scalar field as the matter source, and it will continue to provide the "relational" or "internal" time à la Leibniz with respect to which other physical quantities of interest —e.g., curvatures, shears, expansion and matter energy density— "evolve". Again, as in the isotropic case, the framework can be further extended to accommodate additional matter fields in a rather straightforward fashion.

[1] In the isotropic case, "improved dynamics" [34] required that $\bar{\mu}$ be proportional to $1/\sqrt{|p|}$. In the anisotropic case, one has three p_i and quantum dynamics requires the introduction of three $\bar{\mu}_i$. In the Bianchi I case now under consideration, it was simply assumed [79, 80, 81, 83] that $\bar{\mu}_i$ be proportional to $1/\sqrt{|p_i|}$. We will see in Sec. 2.3.2 that a more systematic procedure leads to the conclusion that the correct generalization of the isotropic result is more subtle. For example, $\bar{\mu}_1$ is proportional to $\sqrt{|p_1|/|p_2 p_3|}$.

To achieve this goal one has to overcome rather nontrivial obstacles which had stalled progress for the past two years. This requires significant new inputs. The first is conceptual: we will sharpen the correspondence between LQG and LQC that underlies the definition of the curvature operator $\hat{F}_{ab}{}^i$ in terms of holonomies. The holonomies we are led to use in this construction will have a nontrivial dependence on triads, stemming from the choice of loops on which they are evaluated (see footnote 1). As a result, at first it seems very difficult to define the action of the resulting quantum holonomy operators. Indeed this was the primary technical obstacle that forced earlier investigations to take certain short cuts —the assumption mentioned above— when defining $\hat{F}_{ab}{}^i$. The second new input is the definition of these holonomy operators without having to take a recourse to such short cuts. But then the resulting Hamiltonian constraint appears unwieldy at first. The third major input is a rearrangement of configuration variables that makes the constraint tractable both analytically and also for a numerical study of the problem.

Finally, we will find that the resulting Hamiltonian constraint has a striking feature which could provide a powerful new tool in relating the quantum dynamics of more complicated models to that of simpler models. It turns out that, in LQC, there is a well-defined projection from the Bianchi I physical states to the Friedmann physical states which maps the Bianchi I quantum dynamics *exactly* to the isotropic quantum dynamics. Previous investigations of the relation between quantum dynamics of a more complicated model to that of a simpler model generally began with an embedding of the Hilbert space $\mathcal{H}_{\rm Res}$ of the more restricted model in the Hilbert space $\mathcal{H}_{\rm Gen}$ of the more general model (see, e.g., [101, 102, 103]). In generic situations, the image of $\mathcal{H}_{\rm Res}$ under this embedding was not left invariant by the more general dynamics on $\mathcal{H}_{\rm Gen}$. This led to a concern that the physics resulting from first reducing and then quantizing may be completely different from that obtained by quantizing the larger system and regarding the smaller system as its subsystem. The new idea of projecting from $\mathcal{H}_{\rm Gen}$ to $\mathcal{H}_{\rm Res}$ corresponds to "integrating out the degrees of freedom that are inaccessible to the restricted model" while the embedding $\mathcal{H}_{\rm Res}$ into $\mathcal{H}_{\rm Gen}$ corresponds to "freezing by hand" these extra degrees of freedom. Classically, both are equally good procedures and in fact the embedding is generally easier to construct. However, in the present case, one "integrates out" anisotropies to go from the LQC of the Bianchi I models to that of the Friedmann model. This idea was already proposed and used in [77] in a perturbative treatment of anisotropies in a locally rotationally symmetric and diagonal Bianchi I model. We extend that work in that we consider the full quantum dynamics of the diagonal Bianchi I model without additional symmetries and, furthermore, use the analog of the $\bar{\mu}$ scheme in which the quantum constraint is considerably more involved than in the μ_o scheme used in [77]. The fact that the LQC dynamics of the Friedmann model is recovered exactly provides some concrete support for the hope that LQC may capture the essential features of full LQG, as far as the quantum dynamics of the homogeneous, isotropic degree of freedom is concerned.

The material is organized as follows. We will begin in Sec. 2.2 with an outline of the classical dynamics of Bianchi I models. This overview will not be comprehensive as our goal is only to set the stage for the quantum theory which is developed in Sec. 2.3. In Sec. 2.4 we discuss three key properties of quantum dynamics: the projection map mentioned above, agreement of the LQC dynamics with that of the Wheeler-DeWitt theory away from the Planck regime and effective equations. (The isotropic analogs of these effective equations approximate the full LQC dynamics of Friedmann models extremely well.) In Sec. 2.4 we summarize the main results and discuss some of their ramifications.

2.2 Hamiltonian Framework

In this section we will summarize those aspects of the classical theory that will be needed for quantization. For a more complete description of the classical dynamics see, e.g., [73, 79, 80, 81, 104].

Our space-time manifold M will be topologically $\mathbb{R}^4$. As is standard in the literature on Bianchi models, we will restrict ourselves to *diagonal* Bianchi I metrics. Then one can fix Cartesian coordinates τ, x_i on M and express the space-time metric as:

$$ds^2 = -N^2 d\tau^2 + a_1^2\, dx_1^2 + a_2^2\, dx_2^2 + a_3^2\, dx_3^2\,, \tag{2.1}$$

where N is the lapse and a_i are the directional scale factors. Thus, the dynamical degrees of freedom are encoded in three functions $a_i(\tau)$ of time. Bianchi I symmetries permit us to rescale the three spatial coordinates x_i by independent constants. Under $x_i \to \alpha_i x_i$, the directional scale factors transform as[2] $a_i \to \alpha_i^{-1} a_i$. Thus, the numerical value of a directional scale factor, say a_1, is not an observable; only ratios such as $a_1(\tau)/a_1(\tau')$ are. The matter source will be a massless scalar field which will serve as the relational or internal time. Therefore, it is convenient to work with a harmonic time function, i.e., to ask that τ satisfy $\Box\tau = 0$. From now on we will work with this choice.

Since the spatial manifold is noncompact and all fields are spatially homogeneous, to construct a Lagrangian or a Hamiltonian framework one has to introduce an elementary cell $\mathcal{V}$ and restrict all integrations to it [31]. We will choose $\mathcal{V}$ so that its edges lie along the fixed coordinate axis x_i. As in the isotropic case, it is also convenient to fix a fiducial flat metric $\mathring{q}_{ab}$ with line element

$$ds_o^2 = dx_1^2 + dx_2^2 + dx_3^2 \,. \tag{2.2}$$

We will denote by $\mathring{q}$ the determinant of this metric, by L_i the lengths of the three edges of $\mathcal{V}$ as measured by $\mathring{q}_{ab}$, and by $V_o = L_1 L_2 L_3$ the volume of the elementary cell $\mathcal{V}$ also measured using $\mathring{q}_{ab}$. Finally, we introduce fiducial co-triads $\mathring{\omega}_a^i = D_a x^i$ and the triads $\mathring{e}_i^a$ dual to them. Clearly they are adapted to the edges of $\mathcal{V}$ and are compatible with $\mathring{q}_{ab}$ (i.e., satisfy $\mathring{q}_{ab} = \mathring{\omega}_a^i \mathring{\omega}_b^j \delta_{ij}$). As noted above, Bianchi I symmetries allow each of the three coordinates to be rescaled by an independent constant α_i. Under these rescalings, $x_i \to x_i' = \alpha_i x_i$, co-triads transform as $\mathring{\omega}_a'^i = \alpha_i \mathring{\omega}_a^i$, and triads $\mathring{e}_i^a$ are rescaled by inverse powers of α_i. The fiducial metric is transformed to $\mathring{q}_{ab}'$ defined by $ds_o'^2 := \alpha_1^2 dx_1^2 + \alpha_2^2 dx_2^2 + \alpha_3^2 dx_3^2$. *We must ensure that our physical results do not change under these rescalings.* Finally, the physical co-triads are given by $\omega_a^i = a^i \mathring{\omega}_a^i$ and the physical 3-metric q_{ab} is given by $q_{ab} = \omega_a^i \omega_b^j \, \delta_{ij}$.

With these fiducial structures at hand, we can now introduce the phase space. Recall first that in LQG the canonical pair consists of an SU(2) connection A_a^i and a densitized triad E_i^a of weight one. Using the Bianchi I symmetry, from each

[2]Here and in what follows there is no summation over repeated indices if they are all contravariant or all covariant. On the other hand, a covariant index which is contracted with a contravariant one is summed over 1, 2, 3.

gauge equivalence class of these pairs we can select one and only one, given by:

$$A_a^i =: c^i (L^i)^{-1}\, \mathring{\omega}_a^i, \qquad \text{and} \qquad E_i^a \equiv \sqrt{q}\, e_i^a =: p_i L_i V_o^{-1} \sqrt{\mathring{q}}\, \mathring{e}_i^a, \tag{2.3}$$

where c_i, p_i are constants and $q = (p_1 p_2 p_3)\, \mathring{q}\, V_o^{-1}$ is the determinant of the physical spatial metric q_{ab}. *Thus the connections A_a^i are now labelled by three parameters c^i and the triads E_i^a by three parameters p_i.* If p_i are positive, the physical triad e_i^a and the fiducial triad $\mathring{e}_i^a$ have the same orientation. A change in sign of, say, p_1 corresponds to a change in the orientation of the physical triad brought about by the flip $e_1^a \rightarrow -e_1^a$. These flips are gauge transformations because they do not change the physical metric q_{ab}. The momenta p_i are directly related to the directional scale factors, for example

$$p_1 = \mathrm{sgn}(a_1)|a_2 a_3|\, L_2 L_3, \tag{2.4}$$

where we take the directional scale factor a_i to be positive if the triad vector e_i^a is parallel to $\mathring{e}_i^a$ and negative if it is antiparallel. The other relations can be obtained by the obvious permutations. As we will see below, in any solution to the field equations, the connection components c_i are directly related to the time derivatives of a_i.

The factors of L_i in (2.3) ensure that this parametrization is unchanged if the fiducial co-triad, triad and metric are rescaled via $x_i \rightarrow \alpha_i\, x_i$. However, the parametrization does depend on the choice of the cell $\mathcal{V}$. Thus the situation is the same as in the isotropic case [31]. (The physical fields A_a^i and E_i^a are of course insensitive to changes in the fiducial metric *or* the cell.) To evaluate the symplectic structure of the symmetry reduced theory, as in the isotropic case [31], we begin with the expression of the symplectic structure in the full theory and simply restrict the integration to the cell $\mathcal{V}$. The resulting (nonvanishing) Poisson brackets are given by:

$$\{c^i, p_j\} = 8\pi G\gamma\, \delta_j^i\,. \tag{2.5}$$

To summarize, the phase space in the Bianchi I model is six dimensional, coordinatized by pairs c^i, p_i, subject to the Poisson bracket relations (2.5). This description is tied to the choice of the fiducial cell $\mathcal{V}$ but is insensitive to the choice of fiducial triads, co-triads and metrics.

Next, let us consider constraints. The full theory has a set of three constraints: the Gauss, the diffeomorphism and the Hamiltonian constraints. It is straightforward to check that, because we have restricted ourselves to diagonal metrics and fixed the internal gauge, the Gauss and the diffeomorphism constraints are identically satisfied. We are thus left with just the Hamiltonian constraint. Its expression is obtained by restricting the integration in the full theory to the fiducial cell $\mathcal{V}$:

$$\mathcal{C}_H = \mathcal{C}_{\text{grav}} + \mathcal{C}_{\text{matt}} = \int_{\mathcal{V}} N \; (\mathcal{H}_{\text{grav}} + \mathcal{H}_{\text{matt}}) \; \mathrm{d}^3x \tag{2.6}$$

where N is the lapse function and the gravitational and the matter parts of the constraint densities are given by

$$\mathcal{H}_{\text{grav}} = \frac{E^a_i E^b_j}{16\pi G\sqrt{|q|}} \left(\epsilon^{ij}{}_k F_{ab}{}^k - 2(1+\gamma^2) K^i_{[a} K^j_{b]}\right), \qquad \text{and} \tag{2.7}$$

$$\mathcal{H}_{\text{matt}} = \sqrt{q}\, \rho_{\text{matt}}. \tag{2.8}$$

Here γ is the Barbero-Immirzi parameter, $F_{ab}{}^k$ is the curvature of the connection A^i_a, given by

$$F_{ab}{}^k = 2\partial_{[a} A_{b]}{}^k + \epsilon_{ij}{}^k A^i_a A^j_b\,, \tag{2.9}$$

K^i_a is related to the extrinsic curvature K_{ab} via $K^i_a = K_{ab} e^{bi}$ and ρ_{matt} is the energy density of the matter fields. In general, A^i_a is related to K^i_a and the spin connection Γ^i_a defined by the triad e^a_i via $A^i_a = \Gamma^i_a + \gamma K^i_a$. However, because Bianchi I models are spatially flat, $\Gamma^i_a = 0$ in the gauge chosen in (2.3), whence $A^i_a = \gamma K^i_a$. This property and the fact that spatial derivatives of K^i_a vanish by the Bianchi I symmetry leads us to the relation

$$2K^i_{[a} K^j_{b]} = \gamma^{-2} \epsilon^{ij}{}_k F_{ab}{}^k\,. \tag{2.10}$$

Therefore, the gravitational part of the Hamiltonian constraint can be simplified to

$$\mathcal{H}_{\text{grav}} = -\frac{E^a_i E^b_j}{16\pi G \gamma^2 \sqrt{q}}\, \epsilon^{ij}{}_k\, F_{ab}{}^k$$

$$= -\frac{\sqrt{^oq}}{8\pi G\gamma^2\sqrt{p_1p_2p_3}\,V_o}\ \left(p_1p_2c_1c_2 + p_1p_3c_1c_3 + p_2p_3c_2c_3\right). \tag{2.11}$$

Finally, recall that our matter field is a massless scalar field T. The matter energy density of the scalar field T is given by $\rho_{\rm matt} = p_{(T)}^2/2V^2$, where $V = \sqrt{|p_1p_2p_3|}$ is the physical volume of the elementary cell. Our choice of harmonic time τ implies that the lapse function is given by $N = \sqrt{|p_1p_2p_3|}$. With these choices the constraint (2.6) simplifies further,

$$\mathcal{C}_H = \int_{\mathcal{V}} \left(-\frac{E^a_iE^b_jV_o}{16\pi G\gamma^2\sqrt{^oq}}\epsilon_{ij}{}^kF^k_{ab} + \frac{\sqrt{^oq}}{V_o}\frac{p_T^2}{2}\right) d^3x \tag{2.12}$$

$$= -\frac{1}{8\pi G\gamma^2}\left(p_1p_2c_1c_2 + p_1p_3c_1c_3 + p_2p_3c_2c_3\right) + \frac{p_T^2}{2}. \tag{2.13}$$

Physical states of the classical theory lie on the constraint surface $\mathcal{C}_H = 0$. The time evolution of each p_i and c_i is obtained by taking their Poisson bracket with $\mathcal{C}_H$.

$$\frac{{\rm d}p_1}{{\rm d}\tau} = \{p_1, \mathcal{C}_H\} = -8\pi G\gamma\frac{\partial\mathcal{C}_H}{\partial c_1} = \frac{p_1}{\gamma}\left(p_2c_2 + p_3c_3\right); \tag{2.14}$$

$$\frac{{\rm d}c_1}{{\rm d}\tau} = \{c_1, \mathcal{C}_H\} = 8\pi G\gamma\frac{\partial\mathcal{C}_H}{\partial p_1} = \frac{-c_1}{\gamma}\left(p_2c_2 + p_3c_3\right). \tag{2.15}$$

The four other time derivatives can be obtained via permutations. Although the phase space coordinates c^i, p_i themselves depend on the choice of the fiducial cell $\mathcal{V}$, the dynamical equations for A^i_a and E^a_i —and hence also for the physical metric q_{ab} and the extrinsic curvature K_{ab}— that follow from (2.14) and (2.15) *are independent of this choice.*

Combining Eqs. (2.4), (2.14) and (2.15), one finds

$$c_i = \gamma L_i\, V_o^{-1}\left(a_1a_2a_3\right)^{-1}\frac{{\rm d}a_i}{{\rm d}\tau} = \gamma L_i\frac{1}{N}\frac{{\rm d}a_i}{{\rm d}\tau}. \tag{2.16}$$

It is instructive to relate the c_i to the directional Hubble parameters $H_i = {\rm d}\ln a_i/{\rm d}t$ where t *is the proper time*, corresponding to the lapse function $N_{(t)} = 1$. Since t is related to the harmonic time τ via $N{\rm d}\tau = N_{(t)}{\rm d}t$,

$$\frac{\rm d}{{\rm d}t} = \frac{1}{\sqrt{|p_1p_2p_3|}}\ \frac{\rm d}{{\rm d}\tau}. \tag{2.17}$$

Therefore, we have

$$c_i = \gamma L_i \frac{\mathrm{d}a_i}{\mathrm{d}t} = \gamma L_i a_i H_i \tag{2.18}$$

where $L_i a_i$ is the length of the ith edge of $\mathcal{V}$ as measured by the physical metric q_{ab}.

Next, it is convenient to introduce a mean scale factor $a := (a_1 a_2 a_3)^{1/3}$ which encodes the physical volume element but ignores anisotropies. Then, the mean Hubble parameter is given by

$$H := \frac{\mathrm{d}\ln a}{\mathrm{d}t} = \frac{1}{3}\left(H_1 + H_2 + H_3\right), \qquad \text{where as before} \qquad H_i := \frac{\mathrm{d}\ln a_i}{\mathrm{d}t}. \tag{2.19}$$

Squaring Eq. (2.19) and using the implication

$$H_1 H_2 + H_2 H_3 + H_3 H_1 = 8\pi G \rho_{\mathrm{matt}} \tag{2.20}$$

of the Hamiltonian constraint, we obtain the generalized Friedmann equation for Bianchi I space-times,

$$H^2 = \frac{8\pi G}{3}\rho_{\mathrm{matt}} + \frac{\Sigma^2}{a^6}, \tag{2.21}$$

where

$$\Sigma^2 = \frac{a^6}{18}\left[(H_1 - H_2)^2 + (H_2 - H_3)^2 + (H_3 - H_1)^2\right] \tag{2.22}$$

is the shear term. The right hand side of (2.21) brings out the fact that the anisotropic shears $(H_i - H_j)$ contribute to the energy density; they quantify the energy density in the gravitational waves. Using the fact that our matter field has zero anisotropic stress one can show that Σ^2 is a constant of the motion [81]. If the space-time itself is isotropic, then $\Sigma^2 = 0$ and Eq. (2.21) reduces to the usual Friedmann equation for the standard isotropic cosmology. These considerations will be useful in interpreting quantum dynamics and exploring the relation between the Bianchi I and Friedmann quantum Hamiltonian constraints.

Next, let us consider the scalar field T. Because there is no potential for it, its canonically conjugate momentum $p_{(T)}$ is a constant of motion (which, for definiteness, will be assumed to be positive). Therefore, in any solution to the field equations T grows linearly in the harmonic time τ. Thus, although T does not have the physical dimensions of time, it is a good evolution parameter in the classical theory. The form of the quantum Hamiltonian constraint is such that T will also serve as a viable internal time parameter in the quantum theory.

We will conclude with a discussion of discrete 'reflection symmetries' that will play an important role in the quantum theory. (For further details see Appendix A.) In the isotropic case, there is a single reflection symmetry, $\Pi(p) = -p$ which physically corresponds to the orientation reversal $e_i^a \to -e_i^a$ of triads. These are large gauge transformations, under which the metric q_{ab} remains unchanged. The Hamiltonian constraint is invariant under this reflection whence one can, if one so wishes, restrict one's attention just to the sector $p \geq 0$ of the phase space. In the Bianchi I case, we have three reflections Π_i, each corresponding to the flip of one of the triad vectors, leaving the other two untouched (e.g., $\Pi_1(p_1, p_2, p_3) = (-p_1, p_2, p_3)$). As shown in [105], the Hamiltonian flow is left invariant under the action of each Π_i. Therefore, it suffices to restrict one's attention to the positive octant in which all three p_i are nonnegative: dynamics in any of the other seven octants can be easily recovered from that in the positive octant by the action of the discrete symmetries Π_i.

Remark: In the LQC literature on Bianchi I models, a physical distinction has occasionally been made between the fiducial cells $\mathcal{V}$ which are "cubical" with respect to the fiducial metric $\mathring{q}_{ab}$ and those that are "rectangular." (In the former case all L_i are equal.) However, given *any* cell $\mathcal{V}$ one can always find a flat metric in our collection (2.1) with respect to which $\mathcal{V}$ is cubical. Therefore the distinction is unphysical and the hope that the restriction to cubical cells may resolve some of the physical problems faced in [79, 80, 81] was misplaced.

2.3 Quantum Theory

This section is divided into four parts. In the first, we briefly recall quantum kinematics, emphasizing issues that have not been discussed in the literature. In the second, we spell out a simple but well-motivated correspondence between the LQG and LQC quantum states that plays an important role in the definition of the curvature operator $\hat{F}_{ab}{}^k$ in terms of holonomies. However, the paths along which holonomies are evaluated depend in a rather complicated way on the triad (or momentum) operators, whence at first it seems very difficult to define these holonomy operators. In the third subsection we show that geometric considerations provide a natural avenue to overcome these apparent obstacles. The resulting Hamiltonian constraint is, however, rather unwieldy to work with. In the last subsection we make a convenient redefinition of configuration variables to simplify its action. The simplification, in turn, will provide the precise sense in which the singularity is resolved in the quantum theory.

2.3.1 LQC Kinematics

We will summarize quantum kinematics only briefly, for details, see [79, 80, 81]. Let us begin by specifying the elementary functions on the classical phase space which are to have unambiguous analogs in the quantum theory. In LQC this choice is directly motivated by the structure of full LQG [1, 2, 3]. As one might expect from the isotropic case [31, 33], the elementary variables are the three momenta p_i and holonomies $h_i^{(\ell)}$ along edges parallel to the three axis x_i, where ℓL_i is the length of the edge with respect to the fiducial metric $\mathring{q}_{ab}$.[3] These functions are (over)complete in the sense that they suffice to separate points of the phase space. Taking the x_1 axis for concreteness, the holonomy $h_1^{(\ell)}$ has the form

$$h_1^{(\ell)}(c_1, c_2, c_3) = \cos\frac{c_1\ell}{2}\mathbb{I} + 2\sin\frac{c_1\ell}{2}\tau_1, \tag{2.23}$$

where $\mathbb{I}$ is the unit 2×2 matrix and τ_i constitute a basis of the Lie algebra of SU(2), satisfying $\tau^i\tau^j = \frac{1}{2}\epsilon^{ij}{}_k\tau^k - \frac{1}{4}\delta^{ij}\mathbb{I}$. Thus, the holonomies are completely determined by almost periodic functions $\exp(i\ell c_j)$ of the connection; they are called "almost" periodic because ℓ is any real number rather than an integer. In quantum theory, then, elementary operators $\hat{h}_i^{(\ell)}$ and $\hat{p}_i$ are well-defined and our task is to express other operators of physical interest in terms of these elementary ones.

Recall that in the isotropic case it is simplest to specify the gravitational sector of the kinematic Hilbert space in the triad of p representation: it consists of wave functions $\Psi(p)$ which are symmetric under $p \to -p$ and have a finite norm: $||\Psi||^2 =$

[3]More precisely, the dimensionless number ℓ is the length of the edge along which the holonomy is evaluated, measured in the units of the length of the edge of $\mathcal{V}$ parallel to it. Since ℓ is a ratio of lengths, its value does not depend on the fiducial or any other metric.

$\sum_p |\Psi(p)|^2 < \infty$. In the Bianchi I case it is again simplest to describe $\mathcal{H}_{\rm kin}^{\rm grav}$ in the momentum representation. Consider first a *countable* linear combination,

$$|\Psi\rangle = \sum_{p_1,p_2,p_3} \Psi(p_1,p_2,p_3)\,|p_1,p_2,p_3\rangle \quad \text{with} \quad \sum_{p_1,p_2,p_3} |\Psi(p_1,p_2,p_3)|^2 < \infty, \tag{2.24}$$

of orthonormal basis states $|p_1,p_2,p_3\rangle$, where

$$\langle p_1,p_2,p_3\,|\,p_1',p_2',p_3'\rangle = \delta_{p_1\,p_1'}\,\delta_{p_2\,p_2'}\,\delta_{p_3\,p_3'}\,. \tag{2.25}$$

Next, recall that on the classical phase space the three reflections Π_i represent large gauge transformations under which physics does not change. They have a natural induced action $\hat\Pi_i$ on the space of wave functions $\Psi(p_1,p_2,p_3)$. (Thus, for example, $\hat\Pi_1\Psi(p_1,p_2,p_3) = \Psi(-p_1,p_2,p_3)$.) Physical observables commute with $\hat\Pi_i$. Therefore, as in gauge theories, each eigenspace of $\hat\Pi_i$ provides a physical sector of the theory. Since $\hat\Pi_i^2 = \mathbb{I}$, eigenvalues of $\hat\Pi_i$ are ± 1. For definiteness, as in the isotropic case, we will assume that the wave functions $\Psi(p_1,p_2,p_3)$ are symmetric under $\hat\Pi_i$. Thus, the gravitational part $\mathcal{H}_{\rm kin}^{\rm grav}$ of the kinematical Hilbert space is spanned by wave functions $\Psi(p_1,p_2,p_3)$ satisfying

$$\Psi(p_1,p_2,p_3) = \Psi(|p_1|,|p_2|,|p_3|) \tag{2.26}$$

and which have finite norm.

The basis states $|p_1,p_2,p_3\rangle$ are eigenstates of quantum geometry: In the state $|p_1,p_2,p_3\rangle$ the face S_i of the fiducial cell $\mathcal{V}$ orthogonal to the axis x_i has area $|p_i|$. Note that although $p_i \in \mathbb{R}$, the orthonormality holds via Kronecker deltas rather than the usual Dirac distributions; this is why the LQC quantum kinematics is inequivalent to that of the Schrödinger theory used in Wheeler-DeWitt cosmology. Finally, the action of the elementary operators is given by

$$\hat p_1\,|p_1,p_2,p_3\rangle = p_1\,|p_1,p_2,p_3\rangle, \tag{2.27}$$

$$\widehat{\exp i\ell c_1}|p_1,p_2,p_3\rangle = |p_1 - 8\pi\gamma G\hbar\ell,\; p_2,p_3\rangle, \tag{2.28}$$

and similarly for $\hat p_2$, $\widehat{\exp i\ell c_2}$, $\hat p_3$ and $\widehat{\exp i\ell c_3}$.

The full kinematical Hilbert space $\mathcal{H}_{\rm kin}$ will be the tensor product, $\mathcal{H}_{\rm kin} =$

$\mathcal{H}_{\rm kin}^{\rm grav} \otimes \mathcal{H}_{\rm kin}^{\rm matt}$ where, as in the isotropic case, we will set $\mathcal{H}_{\rm kin}^{\rm matt} = L^2(\mathbb{R}, {\rm d}T)$ for the Hilbert space of the homogeneous scalar field T. On $\mathcal{H}_{\rm kin}^{\rm matt}$, the operator $\hat{T}$ will act by multiplication and $\hat{p}_{(T)} := -i\hbar {\rm d}/{\rm d}T$ will act by differentiation. Note that we can also use a "polymer Hilbert space" for $\mathcal{H}_{\rm kin}^{\rm matt}$ spanned by almost periodic functions of T. The quantum Hamiltonian constraint (2.45) will remain unchanged and our construction of the physical Hilbert space will go through as it is [106].

2.3.2 The Curvature Operator $\hat{F}_{ab}{}^k$

To discuss quantum dynamics, we have to construct the quantum analog of the Hamiltonian constraint. Since there is no operator corresponding to the connection coefficients c_i on $\mathcal{H}_{\rm kin}^{\rm grav}$, we cannot use Eq. (2.13) directly. Rather, as in the isotropic case [34], we will return to the expression (2.12) involving curvature $F_{ab}{}^k$. Our task then is to find the operator on $\mathcal{H}_{\rm kin}^{\rm grav}$ corresponding to $F_{ab}{}^k$. As is usual in LQG, the idea is to first express the curvature in terms of our elementary variables — holonomies and triads— and then replace them by their direct quantum analogs. Recall first that, in the classical theory, the a-b component of $F_{ab}{}^k$ can be written in terms of holonomies around a plaquette (i.e., a rectangular closed loop whose edges are parallel to two of the axes x_i):

$$F_{ab}{}^k = 2 \lim_{Ar_\Box \to 0} \ {\rm Tr}\left(\frac{h_{\Box_{ij}} - \mathbb{I}}{Ar_\Box}\, \tau^k\right)\, {}^o\omega_a^i\, {}^o\omega_b^j, \tag{2.29}$$

where $Ar_\Box$ is the area of the plaquette $\Box$ and the holonomy $h_{\Box_{ij}}$ around the plaquette $\Box_{ij}$ is given by

$$h_{\Box_{ij}} = h_j^{(\bar\mu_j)^{-1}}\, h_i^{(\bar\mu_i)^{-1}}\, h_j^{(\bar\mu_j)}\, h_i^{(\bar\mu_i)} \tag{2.30}$$

where $\bar\mu_j\, L_j$ is the length of the jth edge of the plaquette, as measured by the fiducial metric $\mathring{q}_{ab}$. (There is no summation over i, j.) Because the $Ar_\Box$ is shrunk to zero, the limit is not sensitive to the precise choice of the closed plaquette $\Box$. Now, in LQG the connection operator does not exist, whence if we regard the right side of Eq. (2.29) as an operator, the limit fails to converge in $\mathcal{H}_{\rm kin}^{\rm grav}$. The nonexistence of the connection operator is a direct consequence of the underlying diffeomorphism invariance [107] and is intertwined with the fact that the eigenvalues of geometric

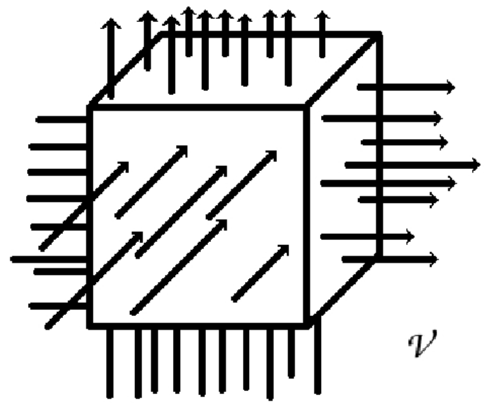

Figure 2.1. Depiction of the LQG quantum geometry state corresponding to the LQC state $|p_1, p_2, p_3\rangle$, with the edges of the spin network traversing through the fiducial cell $\mathcal{V}$. The LQG spin-network has edges parallel to the three axes selected by the diagonal Bianchi I symmetries, each carrying a spin label $j = 1/2$.

operators —such as the area operator $\hat{Ar}_\Box$ associated with the plaquette under consideration— are purely discrete. Therefore, in LQC the viewpoint is that the nonexistence of the limit $Ar_\Box \to 0$ in quantum theory is not accidental: quantum geometry is simply telling us that we should shrink the plaquette not till the area it encloses goes to zero, but rather only to the minimum nonzero eigenvalue $\Delta\, \ell_{\rm Pl}^2$ of the area operator (where Δ is a dimensionless number). The resulting quantum operator $\hat{F}_{ab}{}^k$ then inherits Planck scale nonlocalities.

To implement this strategy in full LQG one must resolve a difficult issue. If the plaquette is to be shrunk only to a finite size, the operator on the right side of Eq. (2.29) would depend on what that limiting plaquette is. So, which of the many plaquettes enclosing an area $\Delta\, \ell_{\rm Pl}^2$ should one use? Without a well-controlled gauge fixing procedure, it would be very difficult to single out such plaquettes, one for each 2-dimensional plane in the tangent space at each spatial point. However, in the diagonal Bianchi I case now under consideration, a natural gauge fixing is available and indeed we have already carried it out. Thus, in the i-j plane, it is natural to choose a plaquette $\Box_{ij}$ so that its edges are parallel to the x_i-x_j axis. Furthermore, the underlying homogeneity implies that it suffices to introduce the three plaquettes at any one point in our spatial 3-manifold.

These considerations severely limit the choice of plaquettes $\Box_{ij}$ but they do not determine the lengths of the two edges in each of these plaquettes. To completely

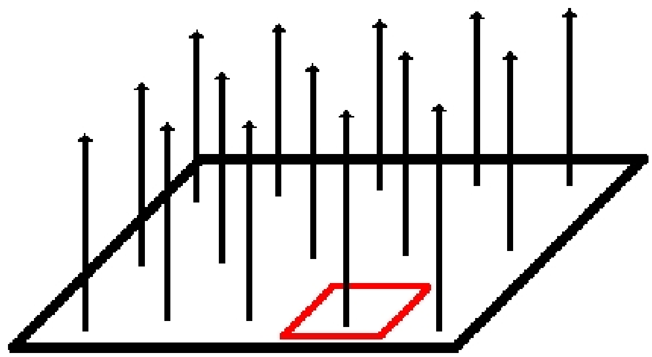

Figure 2.2. Edges of the spin network traversing the 1-2 face of $\mathcal{V}$ and an elementary plaquette associated with a single flux line. This plaquette encloses the smallest quantum of area, $\Delta\,\ell_{\rm Pl}^2$. The curvature operator $\hat{F}_{12}{}^k$ is obtained from the holonomy around such a plaquette.

determine the plaquettes, as in the isotropic case, we will use a simple but well-motivated correspondence between kinematic states in LQG and those in LQC. However, because of anisotropies, new complications arise which require that the correspondence be made much more precise. Fix a state $|p_1, p_2, p_3\rangle$ in $\mathcal{H}_{\rm kin}^{\rm grav}$ of LQC. In this state, the three faces of the fiducial cell $\mathcal{V}$ orthogonal to the x_i-axis have areas $|p_i|$ in the LQC *quantum* geometry. This is the complete physical information in the ket $|p_1, p_2, p_3\rangle$. How would this quantum geometry be represented in full LQG? First, the macroscopic geometry must be spatially homogeneous and we have singled out three axes with respect to which our metrics are diagonal. Therefore, semi-heuristic considerations suggest that the corresponding LQG quantum geometry state should be represented by a spin network consisting of edges parallel to the three axes (see Fig. 2.1). Microscopically this state is not exactly homogeneous. But the *coarse grained* geometry should be homogeneous. To achieve the best possible coarse grained homogeneity, the edges should be packed as tightly as is possible in the desired quantum geometry. That is, each edge should carry the smallest nonzero label possible, namely $j = 1/2$.

For definiteness, let us consider the 1-2 face S_{12} of the fiducial cell $\mathcal{V}$ which is orthogonal to the x_3 axis (see Fig. 2.2). Quantum geometry of LQG tells us that at each intersection of any one of its edges with S_{12}, the spin network contributes a quantum of area $\Delta\,\ell_{\rm Pl}^2$ on this surface, where $\Delta = 4\pi\gamma\sqrt{3}$ [11]. For this LQG state to reproduce the LQC state $|p_1, p_2, p_3\rangle$ under consideration S_{12} must be pierced by N_3 edges of the LQG spin network, where N_3 is given by

$$N_3\,\Delta\,\ell_{\rm Pl}^2 = |p_3|\,.$$

Thus, we can divide S_{12} into N_3 identical rectangles each of which is pierced by exactly one edge of the LQG state, as in Fig. 1(b). Any one of these elementary rectangles encloses an area $\Delta\ell_{\rm Pl}^2$ and provides us the required plaquette $\Box_{12}$. Let the dimensionless lengths of the edges of these plaquettes be $\bar{\mu}_1$ and $\bar{\mu}_2$. Then their lengths with respect to the fiducial metric $\mathring{q}_{ab}$ are $\bar{\mu}_1 L_1$ and $\bar{\mu}_2 L_2$. Since the area of S_{12} with respect to $\mathring{q}_{ab}$ is $L_1 L_2$, we have

$$N_3\;\bar{\mu}_1 L_1\,\bar{\mu}_2 L_2 = L_1 L_2\,.$$

Equating the expressions of N_3 from the last two equations, we obtain

$$\bar{\mu}_1\bar{\mu}_2 = \frac{\Delta\,\ell_{\rm Pl}^2}{|p_3|}\,. \tag{2.31}$$

This relation by itself does not fix $\bar{\mu}_1$ and $\bar{\mu}_2$. However, repeating this procedure for the 2-3 face and the 3-1 face, we obtain in addition two cyclic permutations of this last equation and the three simultaneous equations do suffice to determine $\bar{\mu}_i$:

$$\bar{\mu}_1 = \sqrt{\frac{|p_1|\Delta\,\ell_{\rm Pl}^2}{|p_2 p_3|}}, \quad \bar{\mu}_2 = \sqrt{\frac{|p_2|\Delta\,\ell_{\rm Pl}^2}{|p_1 p_3|}}, \quad \bar{\mu}_3 = \sqrt{\frac{|p_3|\Delta\,\ell_{\rm Pl}^2}{|p_1 p_2|}}\,. \tag{2.32}$$

To summarize, by exploiting the Bianchi I symmetries and using a simple but well-motivated correspondence between LQG and LQC states we have determined the required elementary plaquettes enclosing an area $\Delta\,\ell_{\rm Pl}^2$ on each of the three faces of the cell $\mathcal{V}$. On the face S_{ij}, the plaquette is a rectangle whose sides are parallel to the x_i and x_j axes and whose dimensionless lengths are $\bar{\mu}_i$ and $\bar{\mu}_j$ respectively, given by (2.32). Note that (as in the isotropic case [34]) the $\bar{\mu}_i$ and hence the plaquettes are not fixed once and for all; they depend on the LQC state $|p_1, p_2, p_3\rangle$ of quantum geometry in a specific fashion. The functional form of this dependence is crucial to ensure that the resulting quantum dynamics is free from the difficulties encountered in earlier works.

Components of the curvature operator $\hat{F}_{ab}{}^k$ can now be expressed in terms of holonomies around these plaquettes:

$$\hat{F}_{ab}{}^k = 2 \sum_{i,j} \mathrm{Tr}\left(\frac{h_{\Box_{ij}} - \mathbb{I}}{\bar{\mu}_i \bar{\mu}_j L_i L_j}\, \tau^k\right) {}^o\omega_a^i \, {}^o\omega_b^j, \tag{2.33}$$

with

$$h_{\Box_{ij}} = h_j^{(\bar{\mu}_j)^{-1}}\, h_i^{(\bar{\mu}_i)^{-1}}\, h_j^{(\bar{\mu}_j)}\, h_i^{(\bar{\mu}_i)}\,, \tag{2.34}$$

where $\bar{\mu}_j$ are given by (2.32). (There is no summation over i, j.) Using the expression (2.23) of holonomies, it is straightforward to evaluate the right hand side. One finds:

$$\hat{F}_{ab}{}^k = \epsilon_{ij}{}^k \left(\frac{\sin \bar{\mu} c}{\bar{\mu} L}\, {}^o\omega_a\right)^i \left(\frac{\sin \bar{\mu} c}{\bar{\mu} L}\, {}^o\omega_b\right)^j, \tag{2.35}$$

where the usual summation convention for repeated covariant and contravariant indices applies and

$$\left(\frac{\sin \bar{\mu} c}{\bar{\mu} L}\, \mathring{\omega}_a\right)^i = \frac{\sin \bar{\mu}^i c^i}{\bar{\mu}^i L^i}\, \mathring{\omega}_a^i, \tag{2.36}$$

where there is now no sum over i. This is the curvature operator we were seeking.

We will conclude with a discussion of the important features of this procedure and of the resulting quantum dynamics.

1. In the isotropic case all p_i are equal ($p_i = p$) whence our expressions for $\bar{\mu}_i$ reduce to a single formula, $\bar{\mu} = \sqrt{\Delta \ell_{\mathrm{Pl}}^2/|p|}$. This is precisely the result that was obtained in the "improved dynamics" scheme for the $k = 0$ isotropic models. Thus, we have obtained a generalization of that result to Bianchi I models.

2. In both cases, the key observation is that the plaquette should be shrunk till its area with respect to the physical —rather than the fiducial— geometry is $\Delta\, \ell_{\mathrm{Pl}}^2$. However, there are also some differences. First, in the above analysis we set up and used a correspondence between *quantum* geometries of LQG and LQC in the context of Bianchi I models. In contrast to the previous treatment in the isotropic models [34], we did not have to bring in classical geometry in the intermediate steps. In this sense, even for the isotropic case, the current analysis is an improvement over what is available in the literature.

3. A second difference between our present analysis and that of [34] is the following. Here, the semi-heuristic representation of LQC states $|p_1, p_2, p_3\rangle$ in terms of spin networks of LQG suggested that we should consider spin networks which pierce the faces of the fiducial cell $\mathcal{V}$ as in Fig. 2.1. (As one would expect, these states are gauge invariant.) The minimum nonzero eigenvalue of the area operator on such states is $\Delta\, \ell_{\rm Pl}^2$ with $\Delta = 4\sqrt{3}\pi\gamma$. This is *twice* the absolute minimum nonzero eigenvalue on *all* gauge invariant states. However, that lower value is achieved on spin networks (whose edges are again labelled by $j = 1/2$ but) which do not pierce the surface but rather intersect it from only one side. (In order for the state to be gauge invariant, the edge then has to continue along a direction tangential to the surface. For details, see [11].) Obvious considerations suggest that such states cannot feature in homogeneous models. Since the discussion in the isotropic case invoked a correspondence between LQG and LQC at a rougher level, this point was not noticed and the value of Δ used in [34] was $2\sqrt{3}\pi\gamma$. We emphasize, however, that although the current discussion is more refined, it is not a self-contained derivation. A more complete analysis may well change this numerical factor again.

4. On the other hand, we believe that the functional dependence of $\bar{\mu}_i$ on p_i is robust[4]: As in the isotropic case this dependence appears to be essential to make quantum dynamics viable. Otherwise quantum dynamics can either depend on the choice of the fiducial cell $\mathcal{V}$ even to leading order, or is physically incorrect because it allows quantum effects to dominate in otherwise "tame" situations, or both. The previous detailed, quantum treatments of the Bianchi I model in LQC did not have this functional dependence because they lacked the correspondence between LQG and LQC we used. Rather, they proceeded by analogy. As we noted above, in the isotropic case there is a single $\bar{\mu}$ and a single p and the two are related by $\bar{\mu} = \sqrt{\Delta\ell_{\rm Pl}^2/|p|}$. The most straightforward generalization of this relation to Bianchi I models is $\bar{\mu}_i = \sqrt{\Delta\ell_{\rm Pl}^2/|p_i|}$. This expression was simply postulated and then used to construct quantum dynamics [79, 80, 81]. The resulting analysis has provided a number of useful technical insights. However, this quantum dynamics suffers from the problems mentioned above [83]. The possibility that the correct generalization

[4]It is possible that some additional effects may become important at the Planck scale, but that would modify the form of the $\bar{\mu}_i$-scheme only in the Planck regime.

of the isotropic results to Bianchi I models may be given by Eq. (2.32) was noted in [78, 108] and in the Appendix C of [81]. However, for reasons explained in the next subsection, construction of the quantum Hamiltonian operator based on Eq. (2.32) was thought not to be feasible. Therefore, this avenue was used only to gain qualitative insights and was not pursued in the full quantum theory.

2.3.3 The Quantum Hamiltonian Constraint

With the curvature operator $\hat{F}_{ab}{}^k$ at hand, it is straightforward to construct the quantum analog of the Hamiltonian constraint given in Eq. (2.6) because the triad operators can be readily constructed from the three $\hat{p}_i$. Ignoring for a moment the factor-ordering issues, the gravitational part of this operator is given by

$$\hat{\mathcal{C}}_{\rm grav} = -\frac{1}{8\pi G\gamma^2\Delta\ell_{\rm Pl}^2}\Big[p_1p_2|p_3|\sin\bar\mu_1c_1\sin\bar\mu_2c_2 + p_1|p_2|p_3\sin\bar\mu_1c_1\sin\bar\mu_3c_3 + |p_1|p_2p_3\sin\bar\mu_2c_2\sin\bar\mu_3c_3\Big] \qquad (2.37)$$

where for simplicity of notation here and in what follows we have dropped hats on p_i and $\sin\bar\mu_ic_i$. To write the action of this operator on $\mathcal{H}_{\rm kin}^{\rm grav}$, it suffices to specify the action of the operators $\exp(i\bar\mu_ic_i)$ on the kinematical states $\Psi(p_1,p_2,p_3)$. The expression (2.32) of $\bar\mu_i$ and the Poisson brackets [see Eq. (2.5)] imply:

$$\exp(\pm i\bar\mu_1c_1) = \exp\Big(\mp 8\pi\gamma\sqrt{\Delta}\,\ell_{\rm Pl}^3\sqrt{\left|\frac{p_1}{p_2p_3}\right|}\,\frac{\rm d}{{\rm d}p_1}\Big)\,, \qquad (2.38)$$

and its cyclic permutations. At first sight this expression seems too complicated to yield a manageable Hamiltonian constraint.

Remark: In the isotropic case, the corresponding expression is simply

$$\exp(\pm i\bar\mu c) = \exp\Big(\mp 8\pi\gamma\sqrt{\Delta}\,\ell_{\rm Pl}^3\sqrt{\left|\frac{1}{p}\right|}\frac{\rm d}{{\rm d}p}\Big)\,.$$

Since $\frac{1}{\sqrt{p}}\frac{\rm d}{{\rm d}p}\sim\frac{\rm d}{{\rm d}v}$, where $v\sim|p|^{3/2}$ is the physical volume of the fiducial cell $\mathcal{V}$, this operator can be essentially written as $\exp({\rm d}/{\rm d}v)$ and acts just as a displacement operator on functions $\Psi(v)$ of v. In the operator in Eq. (2.38) by contrast, all three p_i feature in the exponent. This is why its action was deemed unmanageable. As we noted at the end of Sec. 2.3.2, progress was made [79, 80, 81] by simply postulating an alternative, more manageable expression $\bar{\mu}_i = (\sqrt{\Delta}\,\ell_{\rm Pl}/\sqrt{|p_i|})$, the obvious analog of $\bar{\mu} = (\sqrt{\Delta}\,\ell_{\rm Pl})/\sqrt{|p|}$ in the isotropic case [34]. Then each $\exp(\pm i\bar{\mu}_i c_i)$ can be expressed essentially as a displacement operator $\exp \mathrm{d}/\mathrm{d}v_i$ with $v_i \sim |p_i|^{3/2}$ and the procedure used in the isotropic case could be implemented on states $\Psi(v_1, v_2, v_3)$. Bianchi I quantum dynamics then resembled three copies of the isotropic dynamics. However, as noted above this solution is not viable [83].

Our new observation is that the operator (2.38) can in fact be handled in a manageable fashion. Let us first make an algebraic simplification by introducing new dimensionless variables λ_i :

$$\lambda_i \;=\; \frac{\mathrm{sgn}(p_i)\,\sqrt{|p_i|}}{(4\pi\gamma\,\sqrt{\Delta}\,\ell_{\rm Pl}^3)^{1/3}}\,, \tag{2.39}$$

note that $\mathrm{sgn}(\lambda_i) = \mathrm{sgn}(p_i)$. Then, we can introduce a new orthonormal basis $|\lambda_1, \lambda_2, \lambda_3\rangle$ in $\mathcal{H}_{\rm kin}^{\rm grav}$ by an obvious rescaling. These vectors are again eigenvectors of the operators p_i :

$$p_i|\lambda_1, \lambda_2, \lambda_3\rangle \;=\; \mathrm{sgn}(\lambda_i)\,(4\pi\gamma\sqrt{\Delta}\,\ell_{\rm Pl}^3)^{\frac{2}{3}}\,\lambda_i^2\,|\lambda_1, \lambda_2, \lambda_3\rangle\,. \tag{2.40}$$

We can expand out any ket $|\Psi\rangle$ in $\mathcal{H}_{\rm kin}^{\rm grav}$ as $|\Psi\rangle = \Psi(\lambda_1, \lambda_2, \lambda_3)\,|\lambda_1, \lambda_2, \lambda_3\rangle$ and re-express the right side of (2.38) as an operator on wave functions $\Psi(\vec{\lambda})$,

$$\exp(\pm i\bar{\mu}_1 c_1) = \exp\left(\frac{\mp 1}{|\lambda_2\lambda_3|}\,\frac{\mathrm{d}}{\mathrm{d}\lambda_1}\right) =: E_1^{\mp}\,, \tag{2.41}$$

where the notation $E_i^{\pm}$ has been introduced as shorthand. To obtain the explicit action of $E_i^{\pm}$ on wave functions $\Psi(\vec{\lambda})$ we note that, since the operator is an exponential of a vector field, its action is simply to drag the wave function $\Psi(\vec{\lambda})$ a unit affine parameter along its integral curves. Furthermore, since the vector field $\mathrm{d}/\mathrm{d}\lambda_1$ is in the λ_1 direction, the coefficient $1/|\lambda_2\lambda_3|$ is constant along each of its integral curves. Therefore it is possible to write down the explicit expression of

$E_i^{\pm}$:

$$\left(E_1^{\pm}\,\Psi\right)\left(\lambda_1,\lambda_2,\lambda_3\right) \;=\; \Psi\big(\lambda_1 \pm \frac{1}{|\lambda_2\lambda_3|},\lambda_2,\lambda_3\big)\,. \tag{2.42}$$

The nontriviality of this action lies in the fact that while the wave function is dragged along the λ_1 direction, the *affine distance involved in this dragging depends on* λ_2, λ_3. This operator is well-defined because our states have support only on a countable number of λ_i. In particular, the image $\big(E_1^{\pm}\,\Psi\big)(\vec{\lambda})$ vanishes identically at points $\lambda_2 = 0$ or $\lambda_3 = 0$ because Ψ does not have support at $\lambda_1 = \infty$. Thus the factor $\lambda_2\lambda_3$ appearing in the denominator does not cause difficulties.

We can now write out the gravitational part of the Hamiltonian constraint:

$$\hat{\mathcal{C}}_{\rm grav} = \hat{\mathcal{C}}^{(1)}_{\rm grav} + \hat{\mathcal{C}}^{(2)}_{\rm grav} + \hat{\mathcal{C}}^{(3)}_{\rm grav}, \tag{2.43}$$

with

$$\begin{aligned}\hat{\mathcal{C}}^{(1)}_{\rm grav} = &-\frac{\pi\hbar\ell_{\rm Pl}^2}{4}\sqrt{|\lambda_1\lambda_2\lambda_3|}\,\Bigg[\Big(\sin\bar{\mu}_2 c_2\ {\rm sgn}\lambda_2\ + {\rm sgn}\lambda_2\ \sin\bar{\mu}_2 c_2\Big)|\lambda_1\lambda_2\lambda_3| \\ &\times\Big(\sin\bar{\mu}_3 c_3\ {\rm sgn}\lambda_3\ + {\rm sgn}\lambda_3\ \sin\bar{\mu}_3 c_3\Big) + \Big(\sin\bar{\mu}_3 c_3\ {\rm sgn}\lambda_3\ + {\rm sgn}\lambda_3\ \sin\bar{\mu}_3 c_3\Big) \\ &\times|\lambda_1\lambda_2\lambda_3|\Big(\sin\bar{\mu}_2 c_2\ {\rm sgn}\lambda_2 + {\rm sgn}\lambda_2\ \sin\bar{\mu}_2 c_2\Big)\Bigg]\ \sqrt{|\lambda_1\lambda_2\lambda_3|},\end{aligned} \tag{2.44}$$

where we have used a symmetric factor ordering which was first used in [42, 82, 89, 90]. This is a good choice since, as we shall see, the $(\lambda_1,\lambda_2,\lambda_3)$ octants decouple under the action of the Hamiltonian constraint operator for this particular factor ordering. As usual, $\hat{\mathcal{C}}^{(2)}_{\rm grav}$ and $\hat{\mathcal{C}}^{(3)}_{\rm grav}$ are given by the obvious cyclic permutations. In Appendix A we show that, under the action of reflections $\hat{\Pi}_i$ on $\mathcal{H}^{\rm grav}_{\rm kin}$, the operators $\sin\bar{\mu}_i c_i$ have the same transformation properties that c_i have under reflections Π_i in the classical theory. As a consequence, $\hat{\mathcal{C}}_{\rm grav}$ is also reflection symmetric. Therefore, its action is well-defined on $\mathcal{H}^{\rm grav}_{\rm kin}$: $\hat{\mathcal{C}}_{\rm grav}$ is a densely defined, symmetric operator on this Hilbert space. In the isotropic case, its analog has been shown to be essentially self-adjoint [40]. In what follows we will assume that $\hat{\mathcal{C}}_{\rm grav}$ is essentially self-adjoint on $\mathcal{H}^{\rm grav}_{\rm kin}$ and work with its self-adjoint extension.

Finally, it is straightforward to write down the quantum analog of the full

Hamiltonian constraint given in Eq. (2.6):

$$-\hbar^2\partial_T^2\, \Psi(\vec{\lambda}, T) = \hat{\Theta}\, \Psi(\vec{\lambda}, T) \tag{2.45}$$

where $\hat{\Theta} = -\hat{\mathcal{C}}_{\rm grav}$. As in the isotropic case, one can obtain the physical Hilbert space $\mathcal{H}_{\rm phy}$ by a group averaging procedure and the result is completely analogous. Elements of $\mathcal{H}_{\rm phy}$ consist of 'positive frequency' solutions to Eq. (2.45), i.e., solutions to

$$-i\hbar\partial_T\Psi(\vec{\lambda}, T) \;=\; \sqrt{|\hat{\Theta}|}\,\Psi(\vec{\lambda}, T)\,, \tag{2.46}$$

which are symmetric under the three reflection maps $\hat{\Pi}_i$, i.e., satisfy

$$\Psi(\lambda_1, \lambda_2, \lambda_3,\, T) = \Psi(|\lambda_1|, |\lambda_2|, |\lambda_3|,\, T)\,. \tag{2.47}$$

The scalar product is given simply by:

$$\begin{aligned} \langle\Psi_1|\Psi_2\rangle \;&=\; \langle\Psi_1(\vec{\lambda}, T_o)|\Psi_2(\vec{\lambda}, T_o)\rangle_{\rm kin} \\ &=\; \sum_{\lambda_1,\lambda_2,\lambda_3} \bar{\Psi}_1(\vec{\lambda}, T_o)\, \Psi_2(\vec{\lambda}, T_o) \end{aligned} \tag{2.48}$$

where T_o is any "instant" of internal time T.

Remark: In the isotropic LQC literature [34, 46, 47] one began in the classical theory with proper time t (which corresponds to the lapse function $N_{(t)} = 1$) and made a transition to the relational time provided by the scalar field only in the construction of the physical sector of the quantum theory. If we had used that procedure here, the factor ordering of the Hamiltonian constraint would have been slightly different. In this chapter, we started out with the lapse $N = |p_1p_2p_3|^{1/2}$ already in the classical theory because the resulting quantum Hamiltonian constraint is simpler. In the isotropic case, for example, this procedure leads to an *analytically soluble* model (the one obtained in [35] by first starting out with $N_{(t)} = 1$, then going to quantum theory, and finally making some well-motivated but simplifying assumptions). It also has some conceptual advantages because it avoids the use of "inverse scale factors" altogether.

2.3.4 Simplification of $\hat{\mathcal{C}}_{\rm grav}$

It is straightforward to expand out the Hamiltonian constraint $\hat{\mathcal{C}}_{\rm grav}$ using the explicit action of operators $\sin(\bar{\mu}_i c_i)$ given by (2.42) and express it as a linear combination of 24 terms of the type

$$\hat{\mathcal{C}}_{ij}^{\pm\,\pm} := \sqrt{|v|}\, \bar{E}_i^{\pm}\, |v|\, \bar{E}_j^{\pm}\, \sqrt{|v|}\,, \tag{2.49}$$

where $i \neq j$ and we have introduced

$$\bar{E}_i^{\pm} = \frac{1}{2}\Big(E_i^{\pm}{\rm sgn}(\lambda_i) + {\rm sgn}(\lambda_i)E_i^{\pm}\Big). \tag{2.50}$$

Unfortunately, the ${\rm sgn}(\lambda_i)$ factors in this expression and the action of $E_i^{\pm}$ make the result quite complicated. More importantly, it is rather difficult to interpret the resulting operator. The expression can be simplified if we introduce the volume of $\mathcal{V}$ as one of the arguments of the wave function. In particular, this would make quantum dynamics easier to compare with that of the Friedmann models. With this motivation, let us further re-arrange the configuration variables and set

$$v = 2\, \lambda_1 \lambda_2 \lambda_3\,. \tag{2.51}$$

The factor of 2 in Eq. (2.51) ensures that this v reduces to the v used in the isotropic analysis of [34] (if one uses the value of Δ used there). As the notation suggests, v is directly related to the volume of the elementary cell $\mathcal{V}$:

$$\hat{V}\, \Psi(\lambda_1, \lambda_2, v) = 2\pi\, \gamma\, \sqrt{\Delta}\, |v|\, \ell_{\rm Pl}^3\, \Psi(\lambda_1, \lambda_2, v)\,. \tag{2.52}$$

One's first impulse would be to introduce two other variables in a symmetric fashion, e.g., following Misner [109]. Unfortunately, detailed examination shows that they make the constraint even less transparent![5]

[5] Misner-like variables —volume and logarithms of metric components— were used in the brief discussion of Bianchi I models in [78]. This discussion already recognized that the use of volume as one of the arguments of the wave function would lead to simplifications. Dynamics was obtained by starting with the Hamiltonian constraint in the μ_o scheme from [73] and then substituting $\bar{\mu}_i$ of Eq. (2.32) for μ_o^i in the final result. This procedure does simplify the leading order quantum corrections to dynamics. By contrast, our goal is to simplify the full constraint. More importantly, the constraint given in Eq. (2.43) is an improvement over that of [78] because

Let us simply use $(\lambda_1, \lambda_2, v)$ as the configuration variables in place of $(\lambda_1, \lambda_2, \lambda_3)$. This change of variables would be nontrivial in the Schrödinger representation but is completely tame here because the norms on $\mathcal{H}_{\rm kin}^{\rm grav}$ are defined using a discrete measure on $\mathbb{R}^3$. As a consequence, the scalar product is again given by the sum in Eq. (2.48), the only difference is that λ_3 is now replaced by v. Since the choice $(\lambda_1, \lambda_2, v)$ breaks the permutation symmetry, one might have first thought that it would not be appropriate. Somewhat surprisingly, as we will now show, it suffices to make the structure of the constraint transparent. (Of course, the simplification of the constraint would have persisted if we had chosen to replace either λ_1 or λ_2 —rather than λ_3— with v.) Finally, note that the positive octant is now given by $\lambda_1 \geq 0, \lambda_2 \geq 0$ and $v \geq 0$.

To obtain the explicit action of the constraint, it is extremely convenient to use the fact that states Ψ in $\mathcal{H}_{\rm kin}^{\rm grav}$ satisfy the symmetry condition of Eq. (2.47) and that $\hat{\mathcal{C}}_{\rm grav}$ has a well-defined action on this space. Therefore, to specify its action on any given Ψ it suffices to find the restriction of the image $\Phi(\lambda_1, \lambda_2, v) := (\hat{\mathcal{C}}_{\rm grav}\,\Psi)(\lambda_1, \lambda_2, v)$ to the positive octant. The value of Φ in other octants is determined by its symmetry property. *This fact greatly simplifies our task* because we can use it to eliminate the $\mathrm{sgn}(\lambda_i)$ factors in various terms which complicate the expression tremendously.

For concreteness let us focus on one term in the constraint operator (which turns out to be the most nontrivial one for our simplification), leaving the argument as $(\lambda_1, \lambda_2, \lambda_3)$ for this step:

$$\begin{aligned}\Big(\hat{\mathcal{C}}_{21}^{--}\,\Psi\Big)(\lambda_1, \lambda_2, \lambda_3) &= \Big(\sqrt{|v|}\bar{E}_2^-|v|\bar{E}_1^-\sqrt{|v|}\Psi\Big)(\lambda_1, \lambda_2, \lambda_3)\\ &= \Bigg[\sqrt{|v|}|v - 2\,\mathrm{sgn}(\lambda_1\lambda_3)|\sqrt{|v - 2\,\mathrm{sgn}\lambda_3(\mathrm{sgn}\lambda_1 + \mathrm{sgn}\lambda_2^-)|}\\ &\quad\times\Big(\mathrm{sgn}(\lambda_2^-) + \mathrm{sgn}(\lambda_2)\Big)\cdot\Big(\mathrm{sgn}(\lambda_1) + \mathrm{sgn}(\lambda_1 - \tfrac{1}{|\lambda_2^-\lambda_3|})\Big)\Bigg]\\ &\quad\times\ \Psi\Big(\lambda_1 - \tfrac{1}{|\lambda_2^-\lambda_3|}, \lambda_2^-, v - 2\,\mathrm{sgn}\lambda_3(\mathrm{sgn}\lambda_1 + \mathrm{sgn}\lambda_2^-)\Big), \quad (2.53)\end{aligned}$$

we introduced $\bar{\mu}_i$ from the beginning of the quantization procedure and systematically defined the operators $\sin(\bar{\mu}_i c_i)$ (in Sec. 2.3.3).

where we have introduced the shorthand

$$\lambda_2^- = \lambda_2 - \frac{1}{|\lambda_1 \lambda_3|}. \qquad (2.54)$$

If we now restrict the argument of $\left(\hat{\mathcal{C}}_{12}^{--}\,\Psi\right)$ to the positive octant, the expression simplifies to

$$\left(\hat{\mathcal{C}}_{21}^{--}\,\Psi\right)\Big|_{+\,\text{octant}} = \theta_{v-4}\big[\sqrt{v}(v-2)\sqrt{|v-4|}\,\big]\ \Psi\big(\tfrac{v-4}{v-2}\cdot\lambda_1,\ \tfrac{v-2}{v}\cdot\lambda_2,\ v-4\big)\,, \qquad (2.55)$$

where θ_x is the theta function

$$\theta_x = \begin{cases} 0 \text{ if } x \leq 0, \\ 1 \text{ if } x > 0. \end{cases} \qquad (2.56)$$

Now the action of this operator is more transparent: the wave function is multiplied by functions *only* of volume and, in the argument of the wave function, volume simply shifts by -4 and λ_1, λ_2 are rescaled by multiplicative factors which also depend *only* on the volume. Since the full constraint is a linear combination of terms of this form, its action is also driven primarily by volume. As we will see, this key property makes the constraint manageable and greatly simplifies the task of analyzing the relation between the LQC quantum dynamics of the Bianchi I and flat FLRW models. Also note that the presence of the theta function ensures that different octants cannot communicate. From now on, unless otherwise stated, *we will restrict the argument of the images* $\left(\hat{\mathcal{C}}_{ij}^{\pm}\,\Psi\right)$ *to lie in the positive octant*; its value in other octants is given simply by $\left(\hat{\mathcal{C}}_{ij}^{\pm\pm}\,\Psi\right)(\lambda_1, \lambda_2, v) = \left(\hat{\mathcal{C}}_{ij}^{\pm\pm}\,\Psi\right)(|\lambda_1|, |\lambda_2|, |v|)$.

The form (2.55) of the action of operators $\hat{\mathcal{C}}_{ij}^{\pm\pm}$ enables us to discuss singularity resolution. For completeness, let us first write out the four terms corresponding to i, j=1, 2 (which are the most complicated of the 24 terms in $\hat{\mathcal{C}}_{\text{grav}}$):

$$\left(\hat{\mathcal{C}}_{21}^{++}\Psi\right)(\lambda_1, \lambda_2, v) = (v+2)\sqrt{v(v+4)}\cdot\Psi\big(\tfrac{v+4}{v+2}\cdot\lambda_1,\ \tfrac{v+2}{v}\cdot\lambda_2, v+4\big), \qquad (2.57)$$

$$\left(\hat{\mathcal{C}}_{21}^{+-}\Psi\right)(\lambda_1, \lambda_2, v) = v(v+2)\cdot\Psi\big(\tfrac{v}{v+2}\cdot\lambda_1,\ \tfrac{v+2}{v}\cdot\lambda_2, v\big), \qquad (2.58)$$

$$\left(\hat{\mathcal{C}}_{21}^{-+}\Psi\right)(\lambda_1, \lambda_2, v) = \theta_{v-2}\, v(v-2)\cdot\Psi\big(\tfrac{v}{v-2}\cdot\lambda_1,\ \tfrac{v-2}{v}\cdot\lambda_2, v\big), \qquad (2.59)$$

$$\left(\hat{\mathcal{C}}_{21}^{--}\Psi\right)(\lambda_1, \lambda_2, v) = \theta_{v-4}\,(v-2)\sqrt{v|v-4|}\cdot\Psi\big(\tfrac{v-4}{v-2}\cdot\lambda_1,\ \tfrac{v-2}{v}\cdot\lambda_2, v-4\big)\,. \qquad (2.60)$$

Recall that, since v is proportional to the volume of the elementary cell, it vanishes when any one of the three directional scale factors a_i vanish. Thus, the classical singularity corresponds precisely to the points at which v vanishes. Now suppose that the function $\Psi(\lambda_1, \lambda_2, v)$ has no support on points $v = 0$ at an initial internal time T_o. As it evolves via (2.45), can it end up having support on such points? We will argue that this is impossible.

Let us decompose $\mathcal{H}_{\rm kin}^{\rm grav}$ as $\mathcal{H}_{\rm kin}^{\rm grav} = \mathcal{H}_{\rm sing}^{\rm grav} \oplus \mathcal{H}_{\rm reg}^{\rm grav}$ where $\Psi(\lambda_1, \lambda_2, v)$ is in $\mathcal{H}_{\rm sing}^{\rm grav}$ if it has support only on points with $v = 0$ and it is in $\mathcal{H}_{\rm reg}^{\rm grav}$ if it has no support on points with $v = 0$. Now, all the operators $\hat{\mathcal{C}}_{ij}^{\pm\pm}$ have a factor of $\sqrt{v}$ acting on the right (see Eq. (2.49)). It ensures that each $\hat{\mathcal{C}}_{ij}^{\pm\pm}$ annihilates every state in $\mathcal{H}_{\rm sing}^{\rm grav}$. Therefore $\mathcal{H}_{\rm sing}^{\rm grav}$ is left invariant by the evolution. More importantly, because of the pre-factors of $v \pm 2$ and $v \pm 4$ the action of the 4 operators in Eqs. (2.57)–(2.60) preserves $\mathcal{H}_{\rm reg}^{\rm grav}$. This property is shared also by $\hat{\mathcal{C}}_{ij}^{\pm\pm}$ for other values of i, j and hence by $\hat{\mathcal{C}}_{\rm grav}$ and all its powers.[6] Therefore, the relational dynamics of Eq. (2.45) decouples $\mathcal{H}_{\rm sing}^{\rm grav}$ from $\mathcal{H}_{\rm reg}^{\rm grav}$. In particular, if one starts out with a "regular" quantum state at $T = 0$, it remains regular throughout the evolution. In this precise sense, the singularity is resolved.

Next, let us write out explicitly the full Hamiltonian constraint:

$$\begin{aligned}\partial_T^2\, \Psi(\lambda_1, \lambda_2, v; T) = \frac{\pi G}{8}\sqrt{v}\Big[&(v+2)\sqrt{v+4}\,\Psi_4^+(\lambda_1, \lambda_2, v; T)\\ &- (v+2)\sqrt{v}\,\Psi_0^+(\lambda_1, \lambda_2, v; T)\\ &- \theta_{v-2}\,(v-2)\sqrt{v}\,\Psi_0^-(\lambda_1, \lambda_2, v; T)\\ &+ \theta_{v-4}(v-2)\sqrt{|v-4|}\,\Psi_4^-(\lambda_1, \lambda_2, v; T)\Big], \qquad (2.61)\end{aligned}$$

where $\Psi_{0,4}^{\pm}$ are defined as follows:

$$\begin{aligned}\Psi_n^{\pm}(\lambda_1, \lambda_2, v; T) = &\,\Psi\Big(\tfrac{v\pm n}{v\pm 2}\cdot\lambda_1, \tfrac{v\pm 2}{v}\cdot\lambda_2, v\pm n; T\Big) + \Psi\Big(\tfrac{v\pm n}{v\pm 2}\cdot\lambda_1, \lambda_2, v\pm n; T\Big)\\ &+ \Psi\Big(\tfrac{v\pm 2}{v}\cdot\lambda_1, \tfrac{v\pm n}{v\pm 2}\cdot\lambda_2, v\pm n; T\Big) + \Psi\Big(\tfrac{v\pm 2}{v}\cdot\lambda_1, \lambda_2, v\pm n; T\Big)\\ &+ \Psi\Big(\lambda_1, \tfrac{v\pm 2}{v}\cdot\lambda_2, v\pm n; T\Big) + \Psi\Big(\lambda_1, \tfrac{v\pm n}{v\pm 2}\cdot\lambda_2, v\pm n; T\Big). \qquad (2.62)\end{aligned}$$

[6] To make this argument mathematically rigorous one would have to establish that $\hat{\mathcal{C}}_{\rm grav}$ is essentially self-adjoint and its self adjoint extension also shares this property (or a suitable generalization thereof).

As before, we have given the restriction of the image of $\hat{\mathcal{C}}_{\rm grav}$ to the positive octant. Because $\mathcal{H}^{\rm grav}_{\rm reg}$ is left invariant by evolution we can in fact restrict $(\lambda_1, \lambda_2, v)$ to be strictly positive. On the right sides of Eq. (2.62), arguments of Ψ can take negative values, but all such terms will be annihilated by the theta functions in Eq. (2.61). Consequently, knowing the restriction of Ψ to the positive octant, Eqs. (2.61) and (2.62) enable us to directly calculate its image under $\hat{\mathcal{C}}_{\rm grav}$. In particular, numerical evolutions can be carried out by restricting oneself to the positive octant.

Let us now examine the structure of this equation. As in the isotropic case, the right side is a difference equation. As far as the v dependence is concerned, the steps are uniform: the argument of the wave function involves $v-4$, v, $v+4$ exactly as in the isotropic case. The step sizes are also the same as in [34] because, as noted above, our variable v is in precise agreement with that used in the isotropic case. There is again superselection. For each $\epsilon \in [0, 4)$, let us introduce a 'lattice' $\mathcal{L}_\epsilon$ consisting of points $v = 4n + \epsilon$. Then the quantum evolution —as well as the action of the Dirac observables— preserves the subspaces $\mathcal{H}^{\epsilon}_{\rm phy}$ consisting of states with v-support on $\mathcal{L}_\epsilon$. The most interesting of these sectors is the one labelled by $\epsilon = 0$ since it contains the classically singular points where $v = 0$. *Therefore in what follows, unless otherwise stated, we will restrict ourselves to this sector.*

The dependence of $\hat{\mathcal{C}}_{\rm grav}\,\Psi$ on λ_1, λ_2, by contrast, is much more difficult to control technically because the first two arguments of the wave function cannot be chosen to lie on a regular lattice in any simple way. In particular, even if we started out with a wave function which has support only on a lattice, say $\lambda_1 = n\lambda_o$ for some λ_o, the action of $\hat{\mathcal{C}}_{\rm grav}$ shifts support to points such as $\lambda_1 = [(v \pm 2)/v]n\lambda_o$ which do not lie on this lattice. Thus, although there is a superselection sector with respect to λ_1 and λ_2, it is dense in the $\mathbb{R}^2_+$ they span. This point is examined further in Chapter 5 and in [89, 90]. Had it been permissible to set $\bar{\mu}_i \propto /\sqrt{|p_i|}$, we could have restricted λ_i to lie on a regular lattice [79, 80]. Then, following [83], we could have repeated the strategy used successfully in the isotropic case in [35] to simplify dynamics by carrying out a Fourier transform to pass to variables which are conjugate to λ_1 and λ_2. However, as remarked earlier, that choice of $\bar{\mu}_i$ is inadmissible and hence the strategy cannot be repeated in the Bianchi I case. Nonetheless, it is still feasible to carry out numerical simulations. For, if one knows the support of the quantum state at an initial time T_o and the number of time-steps across which one wants to evolve, one can calculate the number of points on an irregular grid in the λ_1-λ_2 plane on which the wave function will have support. It would be interesting to investigate whether the efficient algorithms that have been introduced in the context of regular lattices [110] can be extended to this case.

We will conclude this discussion by noting that it is possible to read off some qualitative features of dynamics from Eqs. (2.61)–(2.62). Since the steps in v of this difference equation are the same as those in the isotropic case, the dynamics of volume —and also of the matter density $\hat{\rho}_{\rm matt}$, since $\hat{p}_{(T)}$ is a constant of motion— would be qualitatively similar to that in the isotropic case. What about anisotropies? The λ_I $(I = 1, 2)$ do not feature in the overall numerical factors in (2.61); they appear only in the argument of the wave functions. Under the action of $\hat{\mathcal{C}}_{\rm grav}$, these arguments get rescaled by factors $(v \pm 4)/(v \pm 2)$, $(v \pm 2)/v$ and $v/(v \pm 2)$. For large volumes, or more precisely low densities, these factors go as $1 + O(\rho_{\rm matt}/\rho_{\rm Pl})$. Hence, to leading order, we will recover of the classical result that $a_1 a_2 a_3 (H_i - H_j)$ are constants, where a_i are the directional scale factors and $H_i := {\rm d} \ln a_i/{\rm d}t$, the directional Hubble parameters. Since quantum corrections go as $\rho/\rho_{\rm Pl}$ they are utterly negligible away from the Planck regime.

In the next section we will discuss three important features of dynamics dictated by Eq. (2.61) which provide significant physical intuition in complementary directions.

2.4 Properties of the LQC Quantum Dynamics

This section is divided into three parts. Since we have used the same general procedure as in the isotropic case it is natural to ask how the quantum dynamics of Eq. (2.61) compares to those in [34]. In the first part we show that there is a natural projection from a dense subspace of the physical Hilbert space of the Bianchi I model to that of the Friedmann model which maps the Bianchi I Hamiltonian constraint operator to that of the Friedmann model. This result boosts confidence in the overall coherence and reliability of the quantization scheme used in LQC. In various isotropic models [34, 43, 44, 45, 46, 48], one can derive certain effective equations. Somewhat surprisingly, for states which are semi-classical at a late initial time, they faithfully capture quantum dynamics throughout the entire evolution, including the bounce. The same considerations lead to effective equations in Bianchi I models which were already analyzed by Chiou and Vandersloot in Appendix C of [81]. In the second subsection we briefly discuss these equations and their consequences. In the third we show that, as in the isotropic case [34, 35], there is a precise sense in which the LQC quantum dynamics reduces to that of the Wheeler-DeWitt theory in the low curvature regime.

2.4.1 Relation to the LQC Friedmann Dynamics

The problem of comparing dynamics of a more general system with that of a restricted, symmetry reduced one has been discussed in the literature in several contexts. In the classical theory, symmetric states often provide symplectic submanifolds $\Gamma_{\rm Res}$ of the more general phase spaces $\Gamma_{\rm Gen}$. Furthermore $\Gamma_{\rm Res}$ are preserved by the dynamics on $\Gamma_{\rm Gen}$. Therefore, it is tempting to repeat the same strategy in the quantum theory. Indeed, sometimes it is possible to find natural subspaces $\mathcal{H}_{\rm Res}$ of states with additional symmetry in the full Hilbert space $\mathcal{H}_{\rm Gen}$ of the more general system. However, generically $\mathcal{H}_{\rm Res}$ is not left invariant by the more general dynamics (see, e.g., [101, 102, 103]). In our case, one can introduce an isotropic subspace of $\mathcal{H}_{\rm Res}$ in the quantum theory based on any given fiducial cell $\mathcal{V}$: isotropic states correspond to wave functions $\Psi(\lambda_1, \lambda_2, v)$ which have support only at points $\lambda_1 = \lambda_2 = (v/2)^{1/3}$. (But note that this subspace is not invariantly defined, it is tied to $\mathcal{V}$!) It is easy to check that the space $\mathcal{H}_{\rm Res}$ of these states is not left invariant by the Bianchi I quantum dynamics.

However, this fact cannot be interpreted as saying that there is no simple relation between the quantum dynamics of the two theories: since restriction to $\mathcal{H}_{\rm Res}$ amounts to a sharp freezing of anisotropic degrees of freedom, in view of the quantum uncertainty principle, this procedure is not well suited to compare the quantum dynamics of the two systems. As pointed out in Sec. 2.1, a better strategy is to integrate out the extra, anisotropic degrees of freedom. This would correspond to a *projection map* from $\mathcal{H}_{\rm Gen}$ to $\mathcal{H}_{\rm Res}$ rather than an embedding of $\mathcal{H}_{\rm Res}$ into $\mathcal{H}_{\rm Gen}$.

Consider first, as an elementary example, a particle moving in $\mathbb{R}^3$. Suppose that the potential depends only on z so that dynamics has a symmetry in the

x, y directions. In the classical theory, there are several natural embeddings of the phase space $\Gamma_{\rm Res}$ into $\Gamma_{\rm Gen}$. For example, we can set $(z, p_z) \to (x{=}x_o,\ y{=}y_o,\ z;\ p_x{=}0,\ p_y{=}0,\ p_z)$ and the Hamiltonian vector field of the full theory is then tangential to the images of each of these embeddings. However, in the quantum theory the Hilbert space $\mathcal{H}_{\rm Gen}$ of the full system is $L^2(\mathbb{R}^3, {\rm d}^3x)$ and there is no natural embedding $\psi(z) \to \Psi(x, y, z)$. The classical strategy would suggest setting $\Psi(x, y, z) = \delta(x, x_o)\,\delta(y, y_o)\psi(z)$ but this is not a normalizable state in $\mathcal{H}_{\rm Gen}$ for any $\psi(z)$. Even if one were to ignore this fact and try to evolve these states, one would find that they are not preserved by the full Hamiltonian operator $\hat{H}$.

Note however that there *is* a natural projection $\hat{\mathbb{P}}$ from a dense subspace in $\mathcal{H}_{\rm Gen}$ to that in $\mathcal{H}_{\rm Res}$:

$$\Psi(x, y, z) \;\to\; (\hat{\mathbb{P}}\Psi)(z) := \int dx \int dy\, \Psi(x, y, z) \;\equiv\; \psi(z)\,. \tag{2.63}$$

(For example, we can choose the dense subspace to be the space of smooth functions of compact support.) Furthermore, under this projection, the Hamiltonian operator

$$\hat{H} = -(\hbar^2/2m)\Delta + V(z)$$

of the general system is mapped to the Hamiltonian operator

$$\hat{h} := -(\hbar^2/2m)\frac{{\rm d}^2}{{\rm d}z^2} + V(z)$$

of the reduced system. Hence solutions $\Psi(\vec{x}, t)$ of the Schrödinger equation of the full system are mapped to solutions $\psi(z, t)$ of the reduced system. Finally, this projection strategy continues to work for more general Hamiltonians of the type $f^i(z)p_i + V(z)$ which again have a symmetry in the x, y directions.

Let us return to the Bianchi I model and define a projection $\hat{\mathbb{P}}$ from states $\Psi(\lambda_1, \lambda_2, v)$ of the Bianchi I model to the states $\psi(v)$ of the Friedmann model of [34] as follows:

$$\Psi(\lambda_1, \lambda_2, v) \;\to\; (\hat{\mathbb{P}}\Psi)(v) := \sum_{\lambda_1, \lambda_2} \Psi(\lambda_1, \lambda_2, v) \equiv \psi(v)\,. \tag{2.64}$$

(The idea of using such a map already appeared in [77] where the map was defined between elements of $\text{Cyl}^\star$ of the locally rotationally symmetric Bianchi I model and that of the Friedmann model.) Again, $\hat{\mathbb{P}}$ is a well-defined projection from a dense subspace of the Bianchi I Hilbert space to a dense subspace of the Friedmann Hilbert space consisting, for example, of states which have support only on a finite number of points. As is manifest from Eq. (2.64), its effect is to focus on volume by "integrating out" the anisotropic degrees of freedom with the same volume. Applying this projection map $\hat{\mathbb{P}}$ to Eq. (2.61), we find

$$\begin{aligned}\partial_T^2\psi(v;T) = \frac{3\pi G}{4}\Big[&(v+2)\sqrt{v(v+4)}\psi(v+4;T) - (1+\theta_{v-2})v^2\psi(v;T) \\ &+ \theta_{v-4}(v-2)\sqrt{v(v-4)}\psi(v-4;T)\Big]. \end{aligned} \tag{2.65}$$

This is *precisely* the quantum constraint describing the LQC dynamics of the Friedmann model with lapse[7] $N = |p|^{3/2}$. The reason for the exact agreement is two-fold. First, the Hamiltonian constraint $\hat{\mathcal{C}}_{\text{grav}}$ of the Bianchi I model is a difference operator whose coefficients depend *only* on v and, second, the shift in the argument is dictated *only* by v. Thus, conceptually, λ_1, λ_2 are "inert directions" in the same sense that x, y are in the elementary example discussed above. To summarize, there is a simple —and *exact*— relation between quantum dynamics of the two theories.

In completely general situations, of course, this exact agreement will not persist: the projected dynamics will provide extremely nontrivial corrections to the dynamics of the simpler system. However, the BKL conjecture says that the dynamics of general relativity greatly simplifies near space-like singularities: In this regime, the time evolution at any one spatial point is well modelled by that of Bianchi I cosmology. Therefore, in a large class of situations there may well be a sense in which the quantum dynamics in the deep Planck regime can be projected to that of the Friedmann model with only small corrections. If so, the Planck scale quantum dynamics of the isotropic, homogeneous degree of freedom in the full theory will be much simpler than what one would have a priori expected.

[7]Of course, this assumes that one uses the same lapse and factor-ordering choices in the isotropic case as what we have done here. Compare, e.g., to [42].

2.4.2 Effective Equations

Physically, the most interesting quantum states are those that are sharply peaked at a classical trajectory at late times. As explained in Sec. 2.1, in the isotropic case such states remain peaked at certain effective trajectories at *all times*, including the epoch during which the universe undergoes a quantum bounce. Thus, even in the deep Planck regime quantum physics is well captured by a smooth metric although its dynamics can no longer be approximated by the classical Einstein's equations and its components now contain large, $\hbar$-dependent terms. The effective equations obeyed by these geometries were first derived using ideas from geometrical quantum mechanics [37, 38]. However, the assumptions made in these derivations break down in the deep Planck regime. Therefore a priori there was no reason to expect these equations to describe quantum dynamics so well also in the Planck regime. That they do was first shown by numerical simulations of the exact quantum equations [33, 34] in the k=0, Λ=0 case. It was then realized that this model is in fact exactly soluble [35, 111] and the power of the effective equations could be attributed to this property. However, k=0 models with nonzero cosmological constant and the closed k=1 models do not appear to be exactly soluble. Yet, numerical solutions of the exact quantum equations show that the effective equations continue to capture full quantum dynamics extremely well [43, 44, 46].

New light was shed on this phenomenon by recent work on a path integral formulation of quantum cosmology [60, 61, 62, 64]. The idea here is to return to the original derivation of path integrals due to Feynman and Hibbs [112] starting from quantum mechanics. In the isotropic case, then, the strategy is to *begin* with the kinematics and dynamics of LQC and then rewrite the transition amplitudes as path integrals. The resulting framework has several novel features. First, because the LQC kinematics relies on quantum geometry, paths that feature in the final integral are different from what one would have naïvely expected from the Wheeler-DeWitt theory. Second, the action that features in the measure is not the Einstein-Hilbert action but contains nontrivial quantum corrections. When expressed in the phase space language, $L = p\dot{q} - H(p, q)$, the "Hamiltonian" H turns out to be precisely the effective Hamiltonian constraint derived in [37, 38], even though this casting of the LQC transition amplitudes in the path integral language is exact and does not pre-suppose that we are away from the Planck regime. Now, in the path integral approach, we have the following general paradigm. Consider the equations obtained by varying the action that appears in the path integral. (Generally these are just the classical equations but in LQC they turn out to be the effective equations of [34, 37, 38, 46].) Fix a path representing a solution to these equations. If the action evaluated along this path is large compared to $\hbar$ then that solution is a good approximation to full quantum dynamics. If one applies this idea to isotropic LQC, one is led to conclude that solutions to the effective equations of [37, 38] should be good approximations to full quantum dynamics also in the k=0, $\Lambda \neq 0$ and k=1 cases. This is precisely what one finds in numerical simulations. Thus, the path integral approach may well provide a deeper explanation of the power of effective equations. While numerical simulations are yet to be carried out in detail in the anisotropic case, because of the situation in the simpler cases it is of interest to find analogous effective equations and study their implications.

This task was carried out already by Chiou and Vandersloot in the Appendix C of [81]. We will summarize the relevant results and briefly comment on the general picture that emerges.

Without loss of generality, we can restrict ourselves to the positive octant. Then the effective Hamiltonian constraint is given simply by the direct classical analog of Eq. (2.37):

$$\frac{1}{2}p_{(T)}^2 + \mathcal{C}_{\rm grav}^{\rm eff} = 0 \tag{2.66}$$

where

$$\mathcal{C}_{\rm grav}^{\rm eff} = -\frac{p_1p_2p_3}{8\pi G\gamma^2\Delta}\left[\sin\bar\mu_1c_1\sin\bar\mu_2c_2 + \sin\bar\mu_2c_2\sin\bar\mu_3c_3 + \sin\bar\mu_3c_3\sin\bar\mu_1c_1\right]. \tag{2.67}$$

Since $\sin x$ is bounded by 1 for all x, these equations immediately imply that the matter density, $\rho_{\rm matt} = p_{(T)}^2/2V^2 \equiv p_{(T)}^2/2p_1p_2p_3$ can never become greater than the critical density $\rho_{\rm crit} \approx 0.41\rho_{\rm Pl}$, first found in the isotropic case [34, 35, 39, 46, 48]. Since ρ becomes infinite at the big bang singularity in the classical evolution, there is a precise sense in which the singularity is resolved in the effective theory.

Effective equations are obtained via Poisson brackets as in Sec. 2.2 but using

Eq. (2.66) in place of the classical Hamiltonian constraint. This gives, for example,

$$\frac{dp_1}{d\tau} = \frac{p_1\sqrt{p_1p_2p_3}}{\sqrt{\Delta}\gamma\ell_{\rm Pl}}\,\cos(\bar{\mu}_1c_1)\,\Big(\sin\bar{\mu}_2c_2 + \sin\bar{\mu}_3c_3\Big), \tag{2.68}$$

and

$$\begin{aligned}\frac{dc_1}{d\tau} = -\frac{p_2p_3}{\Delta\gamma\ell_{\rm Pl}^2}\Bigg[&\sin\bar{\mu}_1c_1\sin\bar{\mu}_2c_2 + \sin\bar{\mu}_1c_1\sin\bar{\mu}_3c_3 + \sin\bar{\mu}_2c_2\sin\bar{\mu}_3c_3\\ &+ \frac{\bar{\mu}_1c_1}{2}\cos\bar{\mu}_1c_1\big(\sin\bar{\mu}_2c_2 + \sin\bar{\mu}_3c_3\big)\\ &- \frac{\bar{\mu}_2c_2}{2}\cos\bar{\mu}_2c_2\big(\sin\bar{\mu}_1c_1 + \sin\bar{\mu}_3c_3\big)\\ &- \frac{\bar{\mu}_3c_3}{2}\cos\bar{\mu}_3c_3\big(\sin\bar{\mu}_1c_1 + \sin\bar{\mu}_2c_2\big)\Bigg].\end{aligned} \tag{2.69}$$

Equations for p_2, c_2 and p_3, c_3 are obtained by cyclic permutations. These effective equations include "leading order quantum corrections" to the classical evolution equations (2.14) and (2.15). In any solution, these corrections become negligible in the distant past and in the distant future. As we noted in Sec. 2.2, the shear Σ defined in Eq. (2.22) is a constant of motion in the classical theory. This is no longer the case in the effective theory. However, one can show that it remains finite throughout the evolution, becomes approximately constant in the low curvature region both in the distant past and in the distant future. Furthermore, its value in the distant future is the same as that in the distant past along any effective trajectory in the phase space.

Vandersloot has also carried out numerical integrations of these equations [113]. In the isotropic case each effective trajectory undergoes a quantum bounce when the matter density $\rho_{\rm matt}$ achieves a critical value $\rho_{\rm crit} \approx 0.41\rho_{\rm Pl}$. As one might expect, now the situation is more complicated because of the additional degrees of freedom. First, there are now several distinct "bounces". More precisely, in addition to $\rho_{\rm matt}$ (or the scalar curvature), we now have to keep track of the three Hubble rates H_i which directly control the Weyl curvature. In the backward evolution toward the classical big bang, Einstein's equations approximate the effective equations extremely well until the density of one of the H_i enters the Planck regime. Then the quantum corrections start rising quickly. Their net effect is to dilute the quantity in question. Once the quantity exits the Planck regime as a result of this dilution, quantum geometry effects again become negligible. Thus, as in the isotropic case, one avoids *the ultraviolet-infrared tension [21] because the quantum geometry effects are extremely strong in the Planck regime but die off extremely quickly as the system exits this regime.* Secondly, the "volume" or the "density bounce" occurs when the matter density is lower than $\rho_{\rm crit}$. This is not surprising because what matters is the total energy density and now there is also a contribution from gravitational waves. Finally, although there are distinct "bounces" for density (or scalar curvature) and the H_i (or the Weyl curvature invariants), they all occur near each other in the relational time T.

There are indications that the general scenario provided by effective equations captures the qualitative features of the full quantum evolution. However, the arguments are not conclusive. For conclusive evidence for (or against) this picture, one needs numerical simulations of the exact quantum equations of Sec. 2.3.4 or of the path integral treatment given in [62].

2.4.3 Relation to the Wheeler-DeWitt Dynamics

The quantum dynamics of LQC are governed by a *difference* —rather than a *differential*— equation because of the quantum geometry effects. However, we will now show that, as in the isotropic case [34, 35, 46], the LQC quantum dynamics are well approximated by the Wheeler-DeWitt (WDW) differential equation away from the Planck regime where quantum geometry effects become negligible.

In the WDW theory the directional scale factors, and hence the three λ_i, can assume any real value and it is simpler to work with the three λ_i rather than with $(\lambda_1, \lambda_2, v)$. Let us therefore set $\underline{\Psi}(\lambda_1, \lambda_2, \lambda_3; T) = \Psi(\lambda_1, \lambda_2, v; T)$ and assume that $\underline{\Psi}$ admits a smooth extension to all real values of λ_i. The idea is to pair various terms in Eq. (2.62) for different n in such a way so that two of the three arguments of $\underline{\Psi}$ are the same. For example, one such pair is

$$\underline{\Psi}\left(\tfrac{v+4}{v+2}\cdot\lambda_1, \tfrac{v+2}{v}\cdot\lambda_2, \lambda_3; T\right) \quad \text{and} \quad \underline{\Psi}\left(\tfrac{v}{v+2}\cdot\lambda_1, \tfrac{v+2}{v}\cdot\lambda_2, \lambda_3; T\right). \tag{2.70}$$

Next, let us define $v' = v + 2$ and $\lambda'_2 = v'\lambda_2/(v' - 2)$ so that we have

$$\sqrt{v+4} = \sqrt{v'+2} = \sqrt{\left(\lambda_1 + \frac{1}{\lambda'_2\lambda_3}\right)\lambda'_2\lambda_3}\,. \tag{2.71}$$

Ignoring the common pre-factors in Eq. (2.62), the two paired terms in Eq. (2.70) can be expressed as:

$$\begin{aligned}
&\sqrt{v'+2}\ \underline{\Psi}\big(\lambda_1 + \tfrac{1}{\lambda'_2\lambda_3}, \lambda'_2, \lambda_3; T\big) - \sqrt{v'-2}\ \underline{\Psi}\big(\lambda_1 - \tfrac{1}{\lambda'_2\lambda_3}, \lambda'_2, \lambda_3; T\big) \\
&\quad = \tfrac{2}{\lambda'_2\lambda_3}\,\tfrac{\partial}{\partial\lambda_1}\,\sqrt{v'}\ \underline{\Psi}(\lambda_1, \lambda'_2, \lambda_3; T) + O\big((\tfrac{1}{\lambda'_2\lambda_3})^n\,\tfrac{\partial^n}{\partial\lambda_1^n}\,\sqrt{v'}\,\underline{\Psi}\big) \\
&\quad = \tfrac{4\lambda_1}{v'}\,\tfrac{\partial}{\partial\lambda_1}\sqrt{v'}\,\underline{\Psi}(\lambda_1, \lambda'_2, \lambda_3; T) + O\big((\tfrac{1}{\lambda'_2\lambda_3})^n\,\tfrac{\partial}{\partial\lambda_1^n}\,\sqrt{v'}\,\underline{\Psi}\big)
\end{aligned} \tag{2.72}$$

where $n > 1$. [Notice that the v' in the denominator in front of the partial derivative will cancel the $v + 2$ pre-factor in Eq. (2.61).] One can suitably pair all terms in Eq. (2.62) and express them as differential operators with corrections which are small for large values of λ_i. Let us ignore these corrections —i.e., assume that the $(1/\lambda_i\lambda_j)^n\partial_k^n\sqrt{v}\underline{\Psi}$ is negligible for $n > 1$ because $\underline{\Psi}$ is slowly varying and we are in the low density, large scale-factor regime. Then we find that the LQC Hamiltonian constraint (2.61) reduces to a rather simple differential equation:

$$\begin{aligned}
\partial_T^2\underline{\Psi}(\lambda_1, \lambda_2, \lambda_3; T) = \frac{16\pi G}{\sqrt{v}}\Big[&\lambda_1\lambda_2\frac{\partial}{\partial\lambda_1}\frac{\partial}{\partial\lambda_2} + \lambda_1\lambda_3\frac{\partial}{\partial\lambda_1}\frac{\partial}{\partial\lambda_3} \\
&+ \lambda_2\lambda_3\frac{\partial}{\partial\lambda_2}\lambda_3\frac{\partial}{\partial\lambda_3}\Big]\big(\sqrt{v}\,\underline{\Psi}(\lambda_1, \lambda_2, \lambda_3; T)\big).
\end{aligned} \tag{2.73}$$

This equation can be further simplified by introducing $\sigma_i = \log\lambda_i$ and $\underline{\Phi} = \sqrt{v}\underline{\Psi}$. The result is:

$$\partial_T^2\underline{\Phi}(\sigma_1, \sigma_2, \sigma_3; T) = 16\pi G\Big[\frac{\partial^2}{\partial\sigma_1\partial\sigma_2} + \frac{\partial^2}{\partial\sigma_1\partial\sigma_3} + \frac{\partial^2}{\partial\sigma_2\partial\sigma_3}\Big]\underline{\Phi}(\sigma_1, \sigma_2, \sigma_3; T)\,, \tag{2.74}$$

where v is now given by $2\exp(\sum\sigma_i)$. This is precisely the equation we would have obtained if we had started from the classical Hamiltonian constraint, used the Schrödinger quantization and the "covariant factor ordering" of the constraint as in the WDW theory. Thus, the LQC Hamiltonian constraint reduces to the WDW equation under the assumption that $\underline{\Psi}$ is slowly varying in the sense that

$(1/\lambda_i\lambda_j)^n \partial_k^n \sqrt{v}\underline{\Psi}$ can be neglected for $n > 1$ relative to the term for $n = 1$. Since $(\lambda_i\lambda_j)^2$ is essentially the area of the i-j face of the fiducial cell $\mathcal{V}$ in Planck units, this should be an excellent approximation well away from the Planck regime. However, in the Planck regime itself the terms which are neglected in the LQC dynamics are comparable to the terms which are kept whence, as in the isotropic case, the WDW evolution completely fails to approximate the LQC dynamics.

2.5 Discussion

In this chapter we extended the "improved" LQC dynamics of Friedmann space-times [34] to obtain a coherent quantum theory of Bianchi I models. As in the isotropic case, we restricted the matter source to be a massless scalar field since it serves as a viable relational time parameter (à la Leibniz) both in the classical and quantum theories. However, it is rather straightforward to accommodate additional matter fields in this framework.

To incorporate the Bianchi I model, we had to overcome several significant obstacles. First, using discrete symmetries we showed that to specify dynamics it suffices to focus just on the positive octant. This simplified our task considerably. Second, in Sec. 2.3.2 we introduced a more precise correspondence between LQG and LQC and used it to fix the parameters $\bar{\mu}_i$ that determine the elementary plaquettes, holonomies around which define the curvature operator $\hat{F}_{ab}{}^k$. This procedure led us to the expressions $\bar{\mu}_1^2 = (|p_1|\Delta\,\ell_{\rm Pl}^2)/|p_2p_3|$, etc. They reduce to the expression $\bar{\mu}^2 = (\Delta\,\ell_{\rm Pl}^2)/|p|$ of the isotropic models [34, 46, 48]. But even there, the current reasoning has the advantage that it uses only quantum geometry, avoiding reference to classical areas even in the intermediate steps. However, because of this rather complicated dependence of $\bar{\mu}_i$ on p_i, the task of defining operators $\sin\bar{\mu}_i c_i$ seems hopelessly difficult at first. Indeed, this was the key reason why the earlier treatments [79, 80, 81, 83] took a short cut and simply set $\bar{\mu}_i^2 = (\Delta\,\ell_{\rm Pl}^2)/|p_i|$ by appealing to the relation $\bar{\mu}^2 = (\Delta\,\ell_{\rm Pl}^2)/|p|$ in the isotropic case. With this choice, quantization of the Hamiltonian constraint became straightforward and the final Bianchi I quantum theory resembled three copies of that of the Friedmann model. However, this result had the physically unacceptable consequence that significant departures from general relativity could occur in "tame" situations. By a nontrivial extension of the geometrical reasoning used in the isotropic case, in Sec. 2.3.3 we were able to define the operators $\sin \bar{\mu}_i c_i$ for our expressions of $\bar{\mu}_i$. However, the structure of the resulting Hamiltonian constraint turned out to be rather opaque. To simplify its form, in Sec. 2.3.4 we introduced volume as one of the arguments of the wave functions. The action of the gravitational part of the Hamiltonian constraint then became transparent: it turned out to be a difference operator where the multiplicative coefficients in individual terms depend only on volume and the change in the arguments of the wave functions also depends only on volume; individual anisotropies do not feature [see Eqs. (2.61)–(2.62)]. This simplification enabled us to show that the sector $\mathcal{H}^{\rm grav}_{\rm reg}$ of quantum states which have no support on classically singular configurations is preserved by the quantum dynamics. In this precise sense the big bang singularity is resolved. Furthermore, this quantum dynamics is free from the physical drawbacks of the older scheme mentioned above.

In Sec. 2.4 we explored three consequences of quantum dynamics in some detail. First, we showed that there is a projection map $\hat{\mathbb{P}} : \mathcal{H}_{\rm Gen} \to \mathcal{H}_{\rm Res}$ from the Hilbert space of the more general Bianchi I model to that of the more restricted Friedmann model which maps the Bianchi I quantum constraint *exactly* to the Friedmann quantum constraint. This is possible because, as noted above, it is just the volume —rather than the anisotropies— that govern the action of the Bianchi I quantum constraint. This result is of considerable interest because, in view of the BKL conjecture, it suggests that near generic space-like singularities the LQC of Friedmann models may capture qualitative features of the full LQG dynamics of the isotropic, homogeneous degree of freedom. In Sec. 2.4.2 we briefly recalled the effective equations of Chiou and Vandersloot (see Appendix C of [81]). These equations provide intuition for the rich structure of quantum bounces in the Bianchi I model. Their analysis suggests that classical general relativity is an excellent approximation away from the Planck regime. However, in the Planck regime quantum geometry effects rise steeply and forcefully counter the tendency of the classical equations to drive the matter density, the Ricci scalar and Weyl invariants to infinity. (In particular, as in the isotropic case, the matter density is again bounded above by $\rho_{\rm crit} \approx 0.41\rho_{\rm Pl}$.) Thus the quantum geometry effects dilute these quantities and, once the quantity exits the Planck regime, classical general relativity again becomes an excellent approximation. In Sec. 2.4.3 we showed that, as in the isotropic case [34, 35, 46], there is a precise sense in which LQC dynamics is well approximated by that of the WDW theory once quantum geometry effects become negligible.

The rather complicated dependence of $\bar{\mu}_i$ on p_i is also necessary to remove a fundamental conceptual limitation of the older treatments of the Bianchi I model. Recall that, because we have homogeneity and the spatial topology is noncompact, we have to introduce a fiducial cell $\mathcal{V}$ to construct a Lagrangian or a Hamiltonian framework. Of course, the final physical results must be independent of this choice. At first this seems like an innocuous requirement but it turns out to be rather powerful. We will now recall from [83] the argument that this condition is violated with the simpler choice $\bar{\mu}_i^2 = (\Delta\, \ell_{\rm Pl}^2)/|p_i|$ but respected by the more complicated choice we were led to from LQG.

For definiteness, let us fix a fiducial metric $\mathring{q}_{ab}$ and denote by L_i the lengths of the edges of the fiducial cell $\mathcal{V}$. Suppose we were to use a different cell, $\mathcal{V}'$ whose edges have lengths $L_i' = \beta_i L_i$ (no summation over i). Since the basic canonical fields A_a^i and E_i^a are insensitive to the choice of the cell, Eq. (2.3) implies that the labels c_i and p_i we used to characterize them change to $c_1' = \beta_1 c_1$, $p_1' = \beta_2\beta_3 p_1$, etc. The gravitational part of the classical Hamiltonian constraint in Eq. (2.13) is just rescaled by an overall factor $(\beta_1\beta_2\beta_3)^2$ and the inverse symplectic structure is rescaled by $(\beta_1\beta_2\beta_3)^{-1}$. Hence the Hamiltonian vector field is rescaled by $(\beta_1\beta_2\beta_3)$, exactly as it should because the lapse is rescaled by the same factor. Thus, as one would expect, the classical Hamiltonian flow is insensitive to the change $\mathcal{V} \to \mathcal{V}'$. What is the situation in the quantum theory? Physical states belong to the kernel of the Hamiltonian constraint operator $\hat{\mathcal{C}}_H$ whence the two quantum theories will carry the same physics only if $\hat{\mathcal{C}}_H$ is changed at most by an overall rescaling. Analysis is a bit more involved than in the classical case because $\hat{\mathcal{C}}_{\rm grav}$ involves factors of $\sin \bar{\mu}_i c_i$. Now, under $\mathcal{V} \to \mathcal{V}'$, our $\bar{\mu}_i$ transform as $\bar{\mu}_1 \to \bar{\mu}_1' = \beta_1^{-1}\bar{\mu}_1$, whence $\bar{\mu}_1' c_1' = \bar{\mu}_1 c_1$, etc, and the Hamiltonian constraint in Eq. (2.37) is rescaled by an overall multiplicative factor $(\beta_1\beta_2\beta_3)^2$ just as in the classical theory. What happens if we set $\bar{\mu}_i^2 = \Delta\, \ell_{\rm Pl}^2/|p_i|$ as in [79, 80, 81, 83]? Then, we are led to $\bar{\mu}_1' c_1' = (\beta_1/\sqrt{\beta_2\beta_3})\, \bar{\mu}_1 c_1$ etc. Since the constraint in Eq. (2.37) is a sum of terms of the type $p_1 p_2 |p_3| \sin \bar{\mu}_1 c_1\, \sin \bar{\mu}_2 c_2$ it has a rather uncontrolled transformation property and is not simply rescaled by an overall factor. It is then not surprising that, in the Planck regime, the dynamical predictions of the resulting quantum theory (as well as of the effective theory) depend on the choice of the elementary cell. It is rather remarkable that the more complicated form of $\bar{\mu}_i$ that we are led to from LQG kinematics has exactly the right form to make quantum dynamics insensitive to the choice of the fiducial cell $\mathcal{V}$. As mentioned above, it also ensures that the predictions of quantum theory is free of drawbacks of the earlier treatments [79, 80], such as the correlation between the bounce and "directional densities" which do not have an invariant significance.

From physical considerations, as in the isotropic case, it would be most interesting to start at a "late time" with states that are sharply peaked at a classical solution in which the three scale factors assume values for which the curvature is low compared to the Planck scale and $p_{(T)}$ is very large compared to $\hbar$ in classical units $c{=}G{=}1$. One would then evolve these states backward and forward in the "internal" time T. As we just discussed, analytical considerations show that, since the initial wave function is in $\mathcal{H}^{\rm grav}_{\rm reg}$, it will continue to be in that subspace; there is no danger that the expectation values of curvature, anisotropies or density would diverge. But several important questions remain. Are there quantum bounces with a pre-big-bang branch again corresponding to a large, classical universe in the distant past? Is there is a clear distinction between evolutions of data in which there are significant initial anisotropies and data which represent only perturbations on isotropic situations? Even in the second case, do anisotropies grow (or decay) following predictions of the classical theory or are there noticeable deviations because of accumulations of quantum effects over large time periods? Numerical simulations of the LQC equations are essential to provide confidence in the general scenario suggested by effective equations and to supply us with detailed Planck scale physics.

Finally, let us return to full LQG. At the present stage of development, there appears to be considerable freedom in the definition of the quantum Hamiltonian constraint in the full theory. Furthermore, our current understanding of the *physical implications* of these choices is quite limited. Already in the isotropic models, the "improved" dynamics scheme provided some useful lessons: it brought out the fact that these choices can be nontrivially narrowed down by carefully analyzing conceptual issues (e.g., requiring that the physical results should be independent of auxiliary structures introduced in the intermediate steps) and by working out the physical consequences of the theory in detail (to ensure that the quantum geometry effects are not dominant in the low energy regime). Rather innocuous choices —such as those made in arriving at the older μ_o-scheme— can lead to unacceptable consequences on both these fronts [39]. The Bianchi I analysis has sharpened these lessons considerably. The fact that the kinematical interplay between LQG and LQC has a deep impact on the viability of quantum dynamics is especially revealing. A quantum analysis of inhomogeneous perturbations around Bianchi I backgrounds is therefore a promising direction for understanding the physical implications of the choices that have to be made in the definition of the Hamiltonian constraint in full LQG. Such an analysis is likely to narrow down choices and lead us to viable quantization schemes in LQG that lead to good semi-classical behaviour.

Chapter 3

Bianchi Type II Models

3.1 Introduction

In this chapter, we will study the loop quantum cosmology of the Bianchi type II model. These models are of special interest to the issue of singularity resolution because of the intuition derived from the body of results related to the BKL conjecture [71, 72] on the nature of generic, space-like singularities in general relativity (see, e.g., [92]). Specifically, as the system enters the Planck regime, dynamics at any fixed spatial point is expected to be well described by the Bianchi I evolution. However, there are transitions in which the parameters characterizing the specific Bianchi I space-time change and the dynamics of these transitions mimics the Bianchi II time evolution. In the previous chapter, we studied the Bianchi I model in the context of LQC. In this chapter we will extend that analysis to the Bianchi II model. We will follow the same general approach and use the same notation, emphasizing only those points at which the present analysis differs from that of Chapter 2.

Bianchi I and II models are special cases of type A Bianchi models which were analyzed already in the early days of LQC (see in particular [73, 74]). However, as is often the case with pioneering early works, these papers overlooked some important conceptual and technical issues. At the classical level, difficulties faced by the Hamiltonian (and Lagrangian) frameworks in noncompact, homogeneous space-times went unnoticed. In these cases, to avoid infinities, it is necessary to introduce an elementary cell and restrict all integrals to it [31, 34, 114]. The

Hamiltonian frameworks in the early works did not carry out this step. Rather, they were constructed simply by dropping an infinite volume integral (a procedure that introduces subtle inconsistencies). In the quantum theory, the kinematical quantum states were assumed to be periodic —rather than almost periodic— in the connection, and the quantum Hamiltonian constraint was constructed using a "pre-μ_o" scheme. Developments over the intervening years have shown that these strategies have severe limitations (see, e.g., [21, 34, 35, 39, 115]). In this chapter, these limitations will be overcome using ideas and techniques that have been introduced in the isotropic and Bianchi I models in these intervening years. Thus, as in [86], the classical Hamiltonian framework will be based on a fiducial cell, quantum kinematics will be constructed using almost periodic functions of connections and quantum dynamics will use the $\bar{\mu}$ scheme. Nonetheless, the space-time description of Bianchi II models in [73, 74], tailored to LQC, will provide the point of departure of our analysis.

New elements required in this extension from the Bianchi I model can be summarized as follows. Recall first that the spatially homogeneous slices M in Bianchi models are isomorphic to 3-dimensional group manifolds. The Bianchi I group is the 3-dimensional group of translations. Hence the the three Killing vectors $\mathring{\xi}_i^a$ on M —the left invariant vector fields on the group manifold— commute and coincide with the right invariant vector fields $\mathring{e}_i^a$ which constitute the fiducial orthonormal triads on M. In LQC one mimics the strategy used in LQG and spin foams and defines the curvature operator in terms of holonomies around plaquettes whose edges are tangential to these vector fields. The Bianchi II group, on the other hand, is generated by two translations and the rotation on a null 2-plane. Now the Killing vectors $\mathring{\xi}_i^a$ no longer commute and neither do the fiducial triads $\mathring{e}_i^a$. Therefore we have to follow another strategy to build the elementary plaquettes. This situation was already encountered in the k=+1, isotropic models [46, 47]. There, the desired plaquettes can be obtained by alternating between the integral curves of right and left invariant vector fields which do commute. However, in the isotropic case, the gravitational connection is given by $A_a^i = c\, \mathring{\omega}_a^i$, where $\mathring{\omega}_a^i$ are the covectors dual to $\mathring{e}_i^a$ and the holonomies around these plaquettes turned out to be almost periodic functions of the connection component c [46, 47]. By contrast, in the Bianchi II model we have three connection components c^i because of the presence of anisotropies and, unfortunately, the holonomies around our plaquettes are no longer almost periodic functions of c^i. (This is also the case in more complicated Bianchi models.) Since the standard kinematical Hilbert space of LQC consists of almost periodic functions of c^i, these holonomy operators are not well-defined on it. Thus, the strategy [31] used so far in LQC to define the curvature operator is no longer viable.

One could simply enlarge the kinematical Hilbert space to accommodate the new holonomy functions of connections. But then the problem quickly becomes as complicated as full LQG. To solve the problem within the standard, symmetry reduced kinematical framework of LQC, one needs to generalize the strategy to define the curvature operator. Of course, the generalization must be such that, when applied to all previous models, it is compatible with the procedure of computing holonomies around suitable plaquettes used there. We will carry out this task by suitably modifying ideas that have already appeared in the literature. This generalization will enable one to incorporate *all* class A Bianchi models in the LQC framework.

Once this step is taken, one can readily construct the quantum Hamiltonian constraint and the physical Hilbert space, following steps that were introduced in the analysis of the Bianchi I model [86]. But because Bianchi II space-times have spatial curvature, the spin connection compatible with the orthonormal triad is now nontrivial. It leads to two new terms in the Hamiltonian constraint that did not appear in the Bianchi I Hamiltonian. We will analyze these new terms in some detail. In spite of these differences, the big bang singularity is resolved in the same precise sense as in the Bianchi I model [86]: If a quantum state is initially supported only on classically nonsingular configurations, it continues to only be supported on nonsingular configurations throughout its evolution.

This chapter is organized as follows. Section 3.2 summarizes the classical Hamiltonian theory describing Bianchi II models. Section 3.3 discusses the quantum theory. We first define a nonlocal connection operator $\hat{A}_a^i$ and use it to obtain the Hamiltonian constraint. We then show that the singularity is resolved and the Bianchi I quantum dynamics is recovered in the appropriate limit. In Sec. 3.4, we introduce effective equations for the model (with the same caveats as in the Bianchi I case [86]). Finally, in Sec. 3.5 we summarize our results and discuss the new elements that appear in the Bianchi II model.

3.2 Classical Theory

This section is divided into two parts. In the first we recall the structure of Bianchi II space-times and in the second we summarize the phase space formulation, adapted to LQC.

3.2.1 Diagonal Bianchi Type II Space-times

Because the issue of discrete symmetries is subtle in background independent contexts, and because it plays a conceptually important role in the quantum theory of Bianchi II models, we will begin with a brief summary of how various fields are defined [1, 2, 3, 116]. This stream-lined discussion brings out the assumptions which are often only implicit, making the treatment of discrete symmetries clearer.

In the Hamiltonian framework underlying loop quantum gravity (LQG), one fixes an *oriented* 3-manifold M and a 3-dimensional 'internal' vector space I equipped with a positive definite metric q_{ij}. The internal indices $i, j, k, \ldots$ are then freely lowered and raised by q_{ij} and its inverse. A spatial triad e^a_i is an isomorphism from I to the tangent space at each point of M which associates a vector field $v^a := e^a_i v^i$ on M to each vector v^i in I.[1] The dual co-triads are denoted by ω^i_a. Given a triad, we acquire a positive definite metric $q_{ab} := q_{ij}\omega^i_a\omega^j_b$ on M. The metric q_{ab} in turn singles out a 3-form ϵ_{abc} on M which has *positive orientation* and satisfies $\epsilon_{abc}\epsilon_{def}\, q^{ad}q^{be}q^{cf} = 3!$. One can then define a 3-form ϵ_{ijk} on I via $\epsilon_{ijk} = \epsilon_{abc}e^a_i e^b_j e^c_k$. Note that ϵ_{ijk} is automatically compatible with q_{ij}, i.e., $\epsilon_{ijk}\epsilon_{lmn}\, q^{il}q^{jm}q^{kn} = 3!$. If a triad $\bar{e}^a_i$ is obtained by flipping an odd number of the vectors in the triad e^a_i, then $\bar{e}^a_i$ and e^a_i have opposite orientations and the fields they define satisfy $\bar{q}_{ab} = q_{ab}$, $\bar{\epsilon}_{abc} = \epsilon_{abc}$ but $\bar{\epsilon}_{ijk} = -\epsilon_{ijk}$. Had we fixed ϵ_{ijk} once and for all on I, then ϵ_{abc} would have flipped sign under this operation and volume integrals on M computed with the unbarred and barred triads would have had opposite signs. With our conventions, these volume integrals will not change and

[1] Thus, in LQG one begins with nondegenerate triads and metrics, passes to the Hamiltonian framework and then, at the end, extends the framework to allow degenerate geometries.

the parity flips will be symmetries of the symplectic structure and the Hamiltonian constraint.

The triad also determines an unique spin connection Γ^i_a via

$$D_{[a}\omega^i_{b]} \;\equiv\; \partial_{[a}\omega^i_{b]} + \epsilon^i{}_{jk}\Gamma^j_{[a}\omega^k_{b]} \;=\; 0\,. \tag{3.1}$$

The gravitational configuration variable A^i_a is then given by $A^i_a = \Gamma^i_a + \gamma K^i_a$ where $K_{ab} := K^i_a \omega_{bi}$ is the extrinsic curvature of M and γ is the Barbero-Immirzi parameter, representing a quantization ambiguity. (The numerical value of γ is fixed by the black hole entropy calculation.) The momenta E^a_i carry, as usual, density weight 1 and are given by: $E^a_i = \sqrt{q}e^a_i$. The fundamental Poisson bracket is:

$$\{A^i_a(x),\, E^b_j(y)\} = 8\pi G\gamma\; \delta^b_a\, \delta^i_j\, \delta^3(x,y)\,. \tag{3.2}$$

In Bianchi models [104, 117, 118], one restricts oneself to those phase space variables which admit a 3-dimensional group of symmetries which act simply and transitively on M. To avoid a proliferation of spaces and types of indices, it is convenient to identify the internal space I and the Lie-algebra $\mathcal{L}G$ of G via a fixed isomorphism. Then, there is a natural isomorphism $\mathring{\xi}^a_i$ between $\mathcal{L}G \equiv I$ and Killing vector fields on M: for each internal vector v^i, $\mathring{\xi}^a_i v^i$ is a Killing field on M. For brevity we will refer to $\mathring{\xi}^a_i$ as (left invariant) vector fields on M. There is a canonical triad $\mathring{e}^a_i$ —the right invariant vector fields— which is Lie dragged by the $\mathring{\xi}^a_i$. It is convenient to use $\mathring{e}^a_i$ and its dual co-triad $\mathring{\omega}^i_a$ as *fiducial* frames and co-frames. They satisfy:

$$[\mathring{e}_i,\, \mathring{e}_j] = -\mathring{C}^k_{ij}\,\mathring{e}_k, = 0, \qquad \mathrm{d}\,\mathring{\omega}^k = \frac{1}{2}\,\mathring{C}^k_{ij}\mathring{\omega}^i \wedge \mathring{\omega}^j, \tag{3.3}$$

where $\mathring{C}^k_{ij}$ denotes the structure constants of $\mathcal{L}G$.

In the case when G is the Bianchi II group, we have $\mathring{C}^k_{ik} = 0$ as in all class A Bianchi models and, furthermore, the symmetric tensor $k^{kl} := \mathring{C}^k_{ij}\,\epsilon^{ijl}$ has signature +,0,0. Therefore, we can fix, once and for all an orthonormal basis $\mathring{b}^i_1, \mathring{b}^i_2, \mathring{b}^i_3$ in I such that the only nonzero components of $\mathring{C}^k_{ij}$ are

$$\mathring{C}^1_{23} = -\mathring{C}^1_{32} = \tilde{\alpha}\,, \tag{3.4}$$

where $\tilde{\alpha}$ is a nonzero real number[2]. We will assume that this basis is so oriented that

$$\epsilon_{123} := \epsilon_{ijk}\, \mathring{b}_1^i\, \mathring{b}_2^j\, \mathring{b}_3^k \;=\varepsilon, \tag{3.5}$$

where $\varepsilon = \pm 1$ depending on whether the frame e_i^a (which determines the sign of ϵ_{ijk}) is right or left handed. Throughout this chapter we will set $\mathring{\xi}_1^a = \mathring{\xi}_i^a \mathring{b}_1^i$, $\mathring{e}_1^a = \mathring{e}_i^a \mathring{b}_1^i$, $\mathring{\omega}_a^1 = \mathring{\omega}_a^i \mathring{b}_i^1$, etc.

The form of the components of $\mathring{C}_{ij}^k$ in this basis implies that M admits global coordinates x, y, z such that the Bianchi II Killing vectors have the fixed form

$$\mathring{\xi}_1^a = \left(\frac{\partial}{\partial x}\right)^a, \qquad \mathring{\xi}_2^a = \left(\frac{\partial}{\partial y}\right)^a, \qquad \mathring{\xi}_3^a = \tilde{\alpha} y \left(\frac{\partial}{\partial x}\right)^a + \left(\frac{\partial}{\partial z}\right)^a. \tag{3.6}$$

These expressions bring out the fact that, if we were to attempt to compactify the spatial slices to pass to a $\mathbb{T}^3$ topology —as one can in the Bianchi I model— we will no longer have globally well-defined Killing fields. Thus, in the Bianchi II model, we are forced to deal with the subtleties associated with noncompactness of the spatially homogeneous slices.

In the x, y, z chart, the right invariant triad is given by

$$\mathring{e}_1^a = \left(\frac{\partial}{\partial x}\right)^a, \qquad \mathring{e}_2^a = \tilde{\alpha} z \left(\frac{\partial}{\partial x}\right)^a + \left(\frac{\partial}{\partial y}\right)^a, \qquad \mathring{e}_3^a = \left(\frac{\partial}{\partial z}\right)^a, \tag{3.7}$$

and the dual co-triad by

$$\mathring{\omega}_a^1 = (\mathrm{d}x)_a - \tilde{\alpha} z (\mathrm{d}y)_a, \qquad \mathring{\omega}_a^2 = (\mathrm{d}y)_a, \qquad \mathring{\omega}_a^3 = (dz)_a. \tag{3.8}$$

They determine a fiducial 3-metric $\mathring{q}_{ab} := q_{ij} \mathring{\omega}_a^i \mathring{\omega}_b^j$ with Bianchi II symmetries:

$$\mathring{q}_{ab} \mathrm{d}x^a \mathrm{d}x^b = (\mathrm{d}x - \tilde{\alpha} z\, \mathrm{d}y)^2 \,+\, \mathrm{d}y^2 \,+\, \mathrm{d}z^2. \tag{3.9}$$

In the diagonal models, the physical triads e_i^a are related to the fiducial ones

[2]Without loss of generality $\tilde{\alpha}$ can be chosen to be 1. We keep it general because we will rescale it later [see Eq. (3.16)] and because we want to be able to pass to the Bianchi I case by taking the limit $\tilde{\alpha} \to 0$.

by[3]

$$\omega_a^i = a^i(\tau)\mathring{\omega}_a^i \qquad \text{and} \qquad a_i(\tau)e_i^a = \mathring{e}_i^a, \tag{3.10}$$

where the a_i are the three directional scale factors. Since the physical spatial metric is given by $q_{ab} = \omega_a^i \omega_{bi}$, the space-time metric can be expressed as

$$\mathrm{d}s^2 = -N\mathrm{d}\tau^2 + a_1(\tau)^2\,(\mathrm{d}x - \tilde{\alpha}z\,\mathrm{d}y)^2 + a_2(\tau)^2\,\mathrm{d}y^2 + a_3(\tau)^2\,\mathrm{d}z^2 \tag{3.11}$$

where N is the lapse function adapted to the time coordinate τ.

For later use, let us calculate the spin connection determined by the triads e_i^a. From the definition of Γ_a^i in Eq. (3.1) it follows that

$$\Gamma_a^i = -\epsilon^{ijk}\,e_j^b\left(\partial_{[a}\omega_{b]k} + \frac{1}{2}e_k^c\omega_a^l\partial_{[c}\omega_{b]l}\right). \tag{3.12}$$

Using Eq. (3.5), the components of Γ_a^i in the internal basis $\mathring{b}_1^i, \mathring{b}_2^i, \mathring{b}_3^i$ can be expressed as

$$\Gamma_a^1 = \frac{\tilde{\alpha}\varepsilon a_1^2}{2a_2a_3}\,\mathring{\omega}_a^1; \qquad \Gamma_a^2 = -\frac{\tilde{\alpha}\varepsilon a_1}{2a_3}\,\mathring{\omega}_a^2; \qquad \Gamma_a^3 = -\frac{\tilde{\alpha}\varepsilon a_1}{2a_2}\,\mathring{\omega}_a^3. \tag{3.13}$$

Before studying the dynamics of the model, let us examine the action of internal parity transformation Π_k which flips the kth triad vector and leaves the orthogonal vectors alone. (For details see Appendix A and [116]). Under the parity transformation Π_1, for example, we have: $e_1^a \to -e_1^a$, $e_2^a \to e_2^a$, $e_3^a \to e_3^a$ and $a_1 \to -a_1$, $a_2 \to a_2, a_3 \to a_3$ whence $\Gamma_a^1 \to -\Gamma_a^1$, $\Gamma_a^2 \to \Gamma_a^2$, $\Gamma_a^3 \to \Gamma_a^3$. Thus, both e_i^a and Γ_a^i are *proper* internal vectors. ε on the other hand is a pseudo internal scalar, $\varepsilon \to -\varepsilon$ under every Π_k. Note that the fiducial quantities carrying a label o do not change under this transformation; it affects only the physical quantities.

3.2.2 The Bianchi II Phase Space

As is usual in LQC, we will now use the fiducial triads and co-triads to introduce a convenient parametrization of the phase space variables (E_i^a, A_a^i). Since the spatial topology is $\mathbb{R}^3$ and the space is homogeneous, we must introduce a fiducial cell $\mathcal{V}$ and restrict all integrals to it [31, 86, 114]. Because we have restricted ourselves

[3]There is no sum if repeated indices are both covariant or contravariant. As usual, the Einstein summation convention holds if a covariant index is contracted with a contravariant index.

to the diagonal model and these fields are symmetric under the Bianchi II group, from each equivalence class of gauge related phase space variables we can choose a pair of the form

$$E^a_i = \frac{p_i}{V_o} L_i \sqrt{|\mathring{q}|}\mathring{e}^a_i \qquad \text{and} \qquad A^i_a = \frac{c^i}{L^i}\mathring{\omega}^i_a, \tag{3.14}$$

where, as spelled out in footnote 3, there is no sum over i. Note that we have introduced the lengths L_i of the fiducial cell with respect to the fiducial metric $\mathring{q}_{ab}$ as was done in [86]. These variables have direct physical interpretation. For example, p_1 is the (oriented) area of the 2-3 face of the elementary cell with respect to the *physical* metric q_{ab} and $h^{(1)} = \exp c_1\tau_1$ is the holonomy of the *physical* connection A^i_a along the edge of the elementary cell in the x direction.

Thus, a point in the phase space is now coordinatized by six real numbers (p_i, c^i). One can now use the symplectic structure in full general relativity to induce a symplectic structure on our six-dimensional phase space, restricting the integral to the fiducial cell. The nonzero Poisson brackets are given by:

$$\{c^i,\, p_j\} \;=\; 8\pi G\gamma\, \delta^i_j, \tag{3.15}$$

where γ is the Barbero-Immirzi parameter. As in the Bianchi I case, we have a 1-parameter ambiguity in the symplectic structure because of the dependence on V_o in p_i and c_i and we have to make sure that the final physical results are either independent of V_o or remain well-defined as we remove the 'regulator' and take the limit $V_o \to \infty$. Finally, it is convenient to rescale the structure constant in order to simplify the expression of the Hamiltonian constraint; we will set

$$\alpha := \frac{L_2 L_3}{L_1}\tilde{\alpha}\,. \tag{3.16}$$

Our choice in Eq. (3.14) of physical triads and connections has fixed the internal gauge as well as the diffeomorphism freedom. Furthermore, it is easy to explicitly verify that, thanks to Eq. (3.14), the Gauss and the diffeomorphism constraints are automatically satisfied. Thus, as in [86], we are left just with the Hamiltonian constraint

$$\mathcal{C}_H = \int_{\mathcal{V}} \left[\frac{N E^a_i E^b_j}{16\pi G \sqrt{|q|}} \left(\epsilon^{ij}{}_k F_{ab}{}^k - 2(1+\gamma^2) K^i_{[a} K^j_{b]} \right) + N \mathcal{H}_{\text{matt}} \right] \mathrm{d}^3 x \,, \tag{3.17}$$

where $F_{ab}{}^k = 2\partial_{[a} A^k_{b]} + \epsilon_{ij}{}^k A^i_a A^j_b$ is the curvature of A^i_a and $\mathcal{H}_{\text{matt}}$ is the matter Hamiltonian density. As in [86], our matter field will consist only of a massless scalar field T which will later serve as a relational time variable a la Liebniz. (Additional matter fields can be incorporated in a straightforward manner, modulo possible intricacies of essential self-adjointness.) Thus,

$$\mathcal{H}_{\text{matt}} = \frac{1}{2} \frac{p_T^2}{\sqrt{|q|}}. \tag{3.18}$$

Since we want to use the massless scalar field as relational time, it is convenient to use a harmonic-time gauge, i.e., assume that the time coordinate τ in Eq. (3.11) satisfies $\Box\tau = 0$. The corresponding lapse function is $N = \sqrt{|p_1 p_2 p_3|}$. With this choice, the Hamiltonian constraint simplifies considerably. Note first that the extrinsic curvature is given by

$$K^i_a = \gamma^{-1}(A^i_a - \Gamma^i_a).$$

Next, using $p_1 = (\mathrm{sgn} a_1)\, |a_2 a_3|\, L_2 L_3$, etc., the components of the spin connection become:

$$\Gamma^1_a = \frac{\alpha\varepsilon p_2 p_3}{2p_1^2} \frac{\mathring{\omega}^1_a}{L_1}, \qquad \Gamma^2_a = -\frac{\alpha\varepsilon p_3}{2p_1} \frac{\mathring{\omega}^2_a}{L_2}, \qquad \Gamma^3_a = -\frac{\alpha\varepsilon p_2}{2p_1} \frac{\mathring{\omega}^3_a}{L_3}\,. \tag{3.19}$$

Collecting terms, the Hamiltonian constraint in Eq. (3.17) becomes

$$\begin{aligned} \mathcal{C}_H = -\frac{1}{8\pi G \gamma^2} \Big[& p_1 p_2 c_1 c_2 + p_2 p_3 c_2 c_3 + p_3 p_1 c_3 c_1 + \alpha\varepsilon p_2 p_3 c_1 \\ & - (1+\gamma^2) \left(\frac{\alpha p_2 p_3}{2p_1} \right)^2 \Big] + \frac{1}{2} p_T^2 \end{aligned} \tag{3.20}$$

$$= \mathcal{C}_H^{(\mathrm{BI})} - \frac{1}{8\pi G\gamma^2} \Big[\alpha\varepsilon p_2 p_3 c_1 - (1+\gamma^2) \left(\frac{\alpha p_2 p_3}{2p_1} \right)^2 \Big], \tag{3.21}$$

where $\mathcal{C}_H^{(\mathrm{BI})}$ is the Hamiltonian constraint (including the matter term) for Bianchi

I space-times which has already been studied in [86]. Note that this constraint is recovered in the limit $\alpha \to 0$, as it must be.

Knowing the form of the Hamiltonian constraint, it is now possible to derive the time evolution of any classical observable $\mathcal{O}$ by taking its Poisson bracket with $\mathcal{C}_H$:

$$\dot{\mathcal{O}} = \{\mathcal{O}, \mathcal{C}_H\}\,, \tag{3.22}$$

where the 'dot' stands for derivative with respect to harmonic time τ. This gives

$$\dot{p_1} = \gamma^{-1}(p_1p_2c_2 + p_1p_3c_3 + \alpha\varepsilon p_2p_3), \tag{3.23}$$

$$\dot{p_2} = \gamma^{-1}(p_2p_1c_1 + p_2p_3c_3), \tag{3.24}$$

$$\dot{p_3} = \gamma^{-1}(p_3p_1c_1 + p_3p_2c_2), \tag{3.25}$$

$$\dot{c_1} = -\frac{1}{\gamma}\Big(p_2c_1c_2 + p_3c_1c_3 + \frac{1}{2p_1}(1+\gamma^2)\big(\frac{\alpha p_2p_3}{p_1}\big)^2\Big), \tag{3.26}$$

$$\dot{c_2} = -\frac{1}{\gamma}\Big(p_1c_2c_1 + p_3c_2c_3 + \alpha\varepsilon p_3c_1 - \frac{1}{2p_2}(1+\gamma^2)\big(\frac{\alpha p_2p_3}{p_1}\big)^2\Big), \tag{3.27}$$

$$\dot{c_3} = -\frac{1}{\gamma}\Big(p_1c_3c_1 + p_2c_3c_2 + \alpha\varepsilon p_2c_1 - \frac{1}{2p_3}(1+\gamma^2)\big(\frac{\alpha p_2p_3}{p_1}\big)^2\Big). \tag{3.28}$$

Any initial data satisfying the Hamiltonian constraint can be evolved by using the six equations above. It is straightforward to extend these results if there are additional matter fields.

Finally, let us consider the parity transformation Π_k which flips the kth *physical* triad vector e^a_k. (As noted before, this transformation does not act on any of the fiducial quantities which carry a label o.) Under this map, we have: $q_{ab} \to q_{ab}$, $\epsilon_{abc} \to \epsilon_{abc}$ but $\epsilon_{ijk} \to -\epsilon_{ijk}$, $\varepsilon \to -\varepsilon$. The canonical variables c^i, p_i transform as proper internal vectors and co-vectors: For example

$$\Pi_1(c_1, c_2, c_3) \to (-c_1, c_2, c_3) \qquad \text{and} \qquad \Pi_1(p_1, p_2, p_3) \to (-p_1, p_2, p_3)\,. \tag{3.29}$$

Consequently, both the symplectic structure and the Hamiltonian constraint are left invariant under any of the parity maps Π_k.

This Hamiltonian description will serve as the point of departure for loop quantization in the next section.

3.3 Quantum Theory

This section is divided into three parts. In the first, we discuss the kinematics of the model, in the second we define an operator corresponding to the connection A_a^i using holonomies and in the third we introduce the Hamiltonian constraint operator and describe its action on states.

3.3.1 LQC Kinematics

Since the kinematics for the LQC of Bianchi II models is almost identical to that for Bianchi I models we will be brief and we refer the reader to Chapter 2 for further details.

Let us begin by specifying the elementary functions on the classical phase space which will have unambiguous analogs in the quantum theory. As in the Bianchi I model, the elementary variables are the areas p_i and holonomies $h_k^{(\ell)}$ of the gravitational connection A_a^i along the integral curves of $\mathring{e}_k^a$ of length ℓL_k with respect to the fiducial metric $\mathring{q}_{ab}$. These holonomies are given by

$$h_k^{(\ell)}(c_1, c_2, c_3) = \exp\left(\ell c_k \tau_k\right) = \cos\frac{\ell c_k}{2}\mathbb{I} + 2\sin\frac{\ell c_k}{2}\tau_k. \tag{3.30}$$

(Note that ℓ depends on the fiducial cell but not on the fiducial metric.) This family of holonomies is completely determined by the almost periodic functions $\exp(i\ell c_k)$ of the connection. These almost periodic functions will be our elementary configuration variables which will be promoted unambiguously to operators in the quantum theory.

It is simplest to use the p-representation to specify the gravitational sector $\mathcal{H}_{\rm kin}^{\rm grav}$ of the kinematic Hilbert space. The basis is orthonormal in the sense

$$\langle p_1, p_2, p_3 | p_1', p_2', p_3'\rangle = \delta_{p_1 p_1'}\delta_{p_2 p_2'}\delta_{p_3 p_3'}\,, \tag{3.31}$$

where the right side features Kronecker symbols rather than Dirac delta distributions. Kinematical states consist of *countable* linear combinations

$$|\Psi\rangle \;=\; \sum_{p_1,p_2,p_3} \Psi(p_1,p_2,p_3)|p_1,p_2,p_3\rangle \tag{3.32}$$

of these basis states for which the norm

$$||\Psi||^2 = \sum_{p_1,p_2,p_3} |\Psi(p_1,p_2,p_3)|^2 \tag{3.33}$$

is finite.

Next, recall that on the classical phase space the three reflections $\Pi_i : e^a_i \to -e^a_i$ are large gauge transformations under which physics does not change (since both the metric and the extrinsic curvature are left invariant). These large gauge transformations have a natural induced action, denoted by $\hat{\Pi}_i$, on the space of wave functions $\Psi(p_1, p_2, p_3)$. For example,

$$\hat{\Pi}_1 \Psi(p_1,p_2,p_3) = \Psi(-p_1,p_2,p_3). \tag{3.34}$$

Since $\hat{\Pi}_i^2$ is the identity, for each i, the group of these large gauge transformations is simply $\mathbb{Z}_2$. As in Yang-Mills theory, physical states belong to its irreducible representation. For definiteness, as in the isotropic and Bianchi I models, we will work with the symmetric representation. It then follows that $\mathcal{H}^{\rm grav}_{\rm kin}$ is spanned by wave functions $\Psi(p_1, p_2, p_3)$ which satisfy

$$\Psi(p_1,p_2,p_3) = \Psi(|p_1|,|p_2|,|p_3|) \tag{3.35}$$

and have a finite norm.

The action of the elementary operators on $\mathcal{H}^{\rm grav}_{\rm kin}$ is as follows: the momenta act by multiplication whereas the almost periodic functions in c_i shift the ith argument. For example,

$$[\hat{p}_1\Psi](p_1,p_2,p_3) = p_1\,\Psi(p_1,p_2,p_3), \quad \text{and} \tag{3.36}$$

$$\left[\widehat{\exp(i\ell c_1)}\Psi\right](p_1,p_2,p_3) = \Psi(p_1 - 8\pi\gamma G\hbar\ell, p_2, p_3). \tag{3.37}$$

The expressions for $\hat{p}_2, \widehat{\exp(i\ell c_2)}, \hat{p}_3$ and $\widehat{\exp(i\ell c_3)}$ are analogous. Finally, we need to define the operator $\hat{\varepsilon}$ since ε features in the expression of the Hamiltonian constraint. In the classical theory, ε is unambiguously defined on nondegenerate triads, i.e., when $p_1p_2p_3 \neq 0$. In quantum theory, wave functions can have support also on degenerate configurations. We will extend the definition to degenerate triads using the basis $|p_1, p_2, p_3\rangle$:

$$\hat{\varepsilon}\, |p_1, p_2, p_3\rangle := \begin{cases} \ \ |p_1, p_2, p_3\rangle \text{ if } p_1 p_2 p_3 \geq 0, \\ -|p_1, p_2, p_3\rangle \text{ if } p_1 p_2 p_3 < 0. \end{cases} \tag{3.38}$$

Finally, the full kinematical Hilbert space $\mathcal{H}_{\rm kin}$ will be the tensor product $\mathcal{H}_{\rm kin} = \mathcal{H}_{\rm kin}^{\rm grav} \otimes \mathcal{H}_{\rm kin}^{\rm matt}$, where $\mathcal{H}_{\rm kin}^{\rm matt} = L^2(\mathbb{R}, dT)$ is the matter kinematical Hilbert space for the homogeneous scalar field. On $\mathcal{H}_{\rm kin}^{\rm matt}$, $\hat{T}$ will act by multiplication and $\hat{p}_T := -i\hbar \mathrm{d}_T$ will act by differentiation. As in the isotropic and Bianchi I models, our final results would remain unaffected if we use a "polymer representation" also for the scalar field.

3.3.2 The Connection Operator $\hat{A}_a^i$

To define the quantum Hamiltonian constraint, we cannot directly use the symmetry reduced classical constraint in Eq. (3.20) because it contains connection components c_k themselves and in LQC only almost periodic functions of c_k have unambiguous operator analogs. Indeed, in all LQC models considered so far [31, 34, 43, 46, 47, 48, 49, 86], we were led to return to the expression given in Eq. (3.17) in the full theory and mimic the procedure used in LQG [119, 120]. More precisely, the key strategy was to follow full LQG (and spin foams) and define a "field strength operator" using holonomies around suitable closed loops. As mentioned in Sec. 3.1, this strategy no longer works because the required holonomies are no longer almost periodic functions of c_k, whence they fail to yield well-defined operators on the Hilbert space $\mathcal{H}_{\rm kin}^{\rm grav}$. For completeness we will first show this fact explicitly and then introduce a new avenue to bypass this difficulty.

The problematic curvature component turns out to be ${F_{yz}}^1$. To construct the corresponding operator, following the strategy used in the k=+1 case [46, 47], we will introduce a closed loop $\Box_{yz}$ as follows. In the coordinates (x, y, z), i) move from $(0, 0, 0)$ to $(0, \bar{\mu}_2 L_2, 0)$ following $\mathring{\xi}_2^a$; ii) then move from $(0, \bar{\mu}_2 L_2, 0)$ to $(0, \bar{\mu}_2 L_2, \bar{\mu}_3 L_3)$ following $\mathring{e}_3^a$; iii) then move from $(0, \bar{\mu}_2 L_2, \bar{\mu}_3 L_3)$ to $(0, 0, \bar{\mu}_3 L_3)$ following $-\mathring{\xi}_2^a$; and, finally, iv) move from $(0, 0, \bar{\mu}_3 L_3)$ to $(0, 0, 0)$ following $-\mathring{e}_3^a$. The parameters $\bar{\mu}_i$ which determine the 'lengths' of these edges can be fixed by the semi-heuristic correspondence between LQC and LQG exactly as in the Bianchi I model [86] because the geometric considerations used in that analysis continue to hold without any modification in all Bianchi models:

$$\bar{\mu}_1 = \sqrt{\frac{|p_1|\Delta\,\ell_{\rm Pl}^2}{|p_2 p_3|}}, \qquad \bar{\mu}_2 = \sqrt{\frac{|p_2|\Delta\,\ell_{\rm Pl}^2}{|p_1 p_3|}}, \qquad \bar{\mu}_3 = \sqrt{\frac{|p_3|\Delta\,\ell_{\rm Pl}^2}{|p_1 p_2|}}, \tag{3.39}$$

where $\Delta\,\ell_{\rm Pl}^2 = 4\sqrt{3}\pi\gamma\,\ell_{\rm Pl}^2$ is the 'area gap'. The holonomy around this closed loop $\Box_{yz}$ is given by

$$h_{\Box_{yz}} = \frac{2}{c\ \bar{\mu}_2\bar{\mu}_3 L_2 L_3} \cos\left(\frac{\bar{\mu}_2 c_2}{2}\right) \sin\left(\frac{\bar{\mu}_2 c}{2}\right) \Big(c_2 \sin(\bar{\mu}_3 c_3) + \alpha\bar{\mu}_3 c_1 \cos(\bar{\mu}_3 c_3)\Big), \tag{3.40}$$

where

$$c = \sqrt{\alpha^2 \bar{\mu}_3^2 c_1^2 + c_2^2}. \tag{3.41}$$

If we were to shrink the loop so that the area it encloses goes to zero, we do indeed recover the classical expression of ${F_{yz}}^1$. However, because of presence of the term c, if $\alpha \neq 0$ the right side fails to be almost periodic in c_1 and c_2. Hence this holonomy operator fails to exist on $\mathcal{H}_{\rm kin}$. It is clear from the expression (3.41) of c that the problem is independent of the specific way $\bar{\mu}_i$ are fixed.

We will bypass this difficulty by mimicking another strategy used in full LQG [119, 120]: We will use holonomies along segments parallel to $\mathring{e}_i^a$ to define an operator corresponding to the connection itself. This is a natural strategy because holonomies along these segments suffice to separate the Bianchi II connections. Let us set $A_a := A_a^k \tau_k$. Then we have the identity

$$A_a = \lim_{\ell_k \to 0} \sum_k \frac{1}{2\ell_k L_k} \left(h_k^{(\ell_k)} - (h_k^{(\ell_k)})^{-1}\right), \tag{3.42}$$

where $h_k^{(\ell_k)}$ is given by Eq. (3.30). In the expressions of physically interesting operators such as the Hamiltonian constraint of full LQG, one often replaces A_a with the (analog of the) right side of Eq. (3.42). But because of the specific forms of these operators, the limit trivializes on diffeomorphism invariant states of LQG. In LQC, we have gauge fixed the system and therefore cannot appeal to diffeomorphism invariance. Indeed, while the holonomies are well-defined for each nonzero ℓ_k, the limit fails to exist on $\mathcal{H}_{\rm kin}^{\rm grav}$. A natural strategy is to shrink ℓ_k to a judiciously chosen nonzero value. But what would this value be? In the case of plaquettes, we could use the interplay between LQG and LQC directly because the argument p_i of LQC quantum states refers to *quantum* areas of faces of the elementary cell $\mathcal{V}$ [86]. For edges we do not have such direct guidance. There is nonetheless a natural principle one can adopt: normalize ℓ_k such that the numerical coefficient in front of the curvature operator constructed from the resulting connection agrees with that in the expression of the curvature operator constructed from holonomies around closed loops, in all cases where the second construction is available. We will use this strategy. Let us apply it to the Bianchi I model where ${F_{ab}}^k = {\epsilon_{ij}}^k\, A_a^i A_b^j$. Using holonomies around closed loops one obtains the field strength operator

$$\hat{F}_{ab}{}^k = \epsilon_{ij}{}^k \,\big(\frac{\sin\bar{\mu}c}{\bar{\mu}L}\,\mathring{\omega}_a\big)^i\,\big(\frac{\sin\bar{\mu}c}{\bar{\mu}L}\,\mathring{\omega}_b\big)^j \tag{3.43}$$

where

$$\big(\frac{\sin\bar{\mu}c}{\bar{\mu}L}\,\mathring{\omega}_a\big)^i = \big(\frac{\sin\bar{\mu}_i c_i}{\bar{\mu}_i L_i}\,\mathring{\omega}_a^i\big) \qquad \text{(no sum over i)}$$

[see Eqs. (2.35) and (2.36)]. Therefore, our strategy yields $\ell_k = 2\bar{\mu}_k$, that is,

$$\hat{A}_a^k = \frac{\widehat{\sin(\bar{\mu}^k c^k)}}{\bar{\mu}^k L_k}\,\mathring{\omega}_a^k, \tag{3.44}$$

where there is no sum over k. Note that the principle stated above leads us unambiguously to the factor 2 in $\ell_k = 2\bar{\mu}_k$; without recourse to a systematic strategy, one may have naïvely set $\ell_k = \bar{\mu}_k$.

If we compare the expression (3.44) of the connection operator with the expression (3.14) of the classical connection, we have effectively defined an operator $\hat{c}$ via

$$\hat{c}_k = \frac{\widehat{\sin(\bar{\mu}_k c_k)}}{\bar{\mu}_k}, \tag{3.45}$$

where there is again no sum over k. In the literature such a quantization of c is often called "polymerization." Our approach is an improvement over such strategies in two respects. First, we did not just make the substitution $c \to \sin \ell c/\ell$ by hand; a priori one could have used another substitution such as $c \to \tan \ell c/\ell$. Rather, as in full LQG, we used the strategy of expressing the connection in term of holonomies, 'the elementary variables'. But this still leaves open the question of what ℓ one should use. We determined this by requiring that the overall normalization of $\hat{F}_{ab}{}^k$ constructed from $\hat{A}^i_a = c^i (L^i)^{-1} \mathring{\omega}^i_a$ should agree with that of $\hat{F}_{ab}{}^k$ constructed from holonomies around appropriate closed loops, when the second construction is possible. Therefore, our construction is a bona fide generalization of the previous constructions used successfully in LQC.

3.3.2.1 Application to the Open FLRW Model

This strategy has some applications beyond the Bianchi II model studied in this chapter. First, the k=−1 isotropic case has been studied in detail in [48, 49]. The analysis uses the $\bar{\mu}$ scheme, carries out a numerical simulation using exact LQC equations and shows that the effective equations of the "embedding approach" [37, 38] (discussed in Sec. 3.4) provide an excellent approximation to the quantum evolution. While this is an essentially exhaustive treatment, as [48, 49] itself points out, the treatment has a conceptual limitation in that it builds holonomies around the closed loops using the extrinsic curvature K^i_a —rather than A^i_a— as a "connection". This limitation can be overcome easily by using the operator $\hat{A}^i_a$ derived here. In addition, this strategy is applicable to all class A Bianchi models, including type IX. Thus, it opens the door to the LQC treatment of all these models in one go.

3.3.3 The Quantum Hamiltonian Constraint

With the connection operator at hand, one can construct the Hamiltonian constraint operator starting either from the general LQG expression (3.17) or the symmetry reduced expression (3.20). We will begin by a small change in the representation of kinematical states which will facilitate this task.

3.3.3.1 A More Convenient Representation

Ignoring factor ordering ambiguities for the moment, the constraint operator $\hat{\mathcal{C}}_H$ is given by

$$\begin{aligned}\hat{\mathcal{C}}_H = &-\frac{1}{8\pi G\gamma^2\Delta\ell_{\rm Pl}^2}\Big[p_1p_2|p_3|\sin\bar{\mu}_1c_1\sin\bar{\mu}_2c_2+|p_1|p_2p_3\sin\bar{\mu}_2c_2\sin\bar{\mu}_3c_3\\ &+p_1|p_2|p_3\sin\bar{\mu}_3c_3\sin\bar{\mu}_1c_1\Big]-\frac{1}{8\pi G\gamma^2}\Big[\alpha\hat{\varepsilon}p_2p_3\sqrt{\frac{|p_2p_3|}{|p_1|\Delta\ell_{\rm Pl}^2}}\sin\bar{\mu}_1c_1\\ &-(1+\gamma^2)\left(\frac{\alpha p_2p_3}{2p_1}\right)^2\Big]+\frac{1}{2}\hat{p}_T^2,\end{aligned} \tag{3.46}$$

where for simplicity of notation here and in what follows we have dropped the hats on the p_i and $\sin\bar{\mu}_ic_i$ operators. Recall that, classically, the Bianchi II symmetry group reduces to the Bianchi I symmetry group if we set $\alpha = 0$. If one sets $\alpha = 0$ in (3.46), the last two terms disappear and the operator $\hat{\mathcal{C}}_H$ reduces to that of the Bianchi I model [86] showing explicitly that our construction is a natural generalization of the strategy used there.

To obtain the action of operators corresponding to terms of the form $\sin\bar{\mu}_ic_i$ we use the same strategy as in Chapter 2. As shown there, it is simplest to introduce dimensionless variables

$$\lambda_i = \frac{\mathrm{sgn}(p_i)\sqrt{|p_i|}}{(4\pi\gamma\sqrt{\Delta}\ell_{\rm Pl}^3)^{1/3}}. \tag{3.47}$$

Then the kets $|\lambda_1,\lambda_2,\lambda_3\rangle$ constitute an orthonormal basis in which the operators p_k are diagonal

$$p_k|\lambda_1,\lambda_2,\lambda_3\rangle \;=\; [\mathrm{sgn}(\lambda_k)(4\pi\gamma\sqrt{\Delta}\ell_{\rm Pl}^3)^{2/3}\lambda_k^2]\;|\lambda_1,\lambda_2,\lambda_3\rangle\,. \tag{3.48}$$

Quantum states will now be represented by functions $\Psi(\lambda_1,\lambda_2,\lambda_3)$. The operator $e^{i\bar{\mu}_1c_1}$ acts on them as follows

$$\begin{aligned}\big[e^{i\bar{\mu}_1c_1}\,\Psi\big](\lambda_1,\lambda_2,\lambda_3) &= \Psi(\lambda_1-\frac{1}{|\lambda_2\lambda_3|},\lambda_2,\lambda_3)\\ &= \Psi(\frac{v-2\mathrm{sgn}(\lambda_2\lambda_3)}{v}\cdot\,\lambda_1,\lambda_2,\lambda_3),\end{aligned} \tag{3.49}$$

where we have introduced the variable $v = 2\lambda_1\lambda_2\lambda_3$ which is proportional to the volume of the fiducial cell:

$$\hat{V}\,\Psi(\lambda_1,\lambda_2,\lambda_3) \;=\; [2\pi\gamma\sqrt{\Delta}\,|v|\,\ell_{\rm Pl}^3]\,\Psi(\lambda_1,\lambda_2,\lambda_3). \tag{3.50}$$

(The $e^{i\bar{\mu}_1 c_1}$ operator is well-defined in spite of the appearance of $|\lambda_2\lambda_3|$ in the denominator; see Sec. 2.3.3.) The operators $e^{i\bar{\mu}_2 c_2}$ and $e^{i\bar{\mu}_3 c_3}$ have analogous action.

We are now ready to write the Hamiltonian constraint explicitly in the λ_i-representation. As noted above, the three terms in the first square bracket on the right hand side of Eq. (3.46) constitute the gravitational part of $\hat{\mathcal{C}}_H$ for the LQC of Bianchi I model and have been discussed in Chapter 2. In the next two subsections we will now discuss the last two terms which are specific to the Bianchi II model.

3.3.3.2 The Fourth Term in $\hat{\mathcal{C}}_H$

Using a symmetric factor ordering, the fourth term becomes

$$\hat{\mathcal{C}}_H^{(4)} = -\frac{\alpha p_2 p_3\sqrt{|p_2p_3|}}{16\pi G\gamma^2\sqrt{\Delta}\ell_{\rm Pl}}\;\widehat{|p_1|^{-1/4}}\,(\hat{\varepsilon}\,\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_1 c_1\,\hat{\varepsilon})\,\widehat{|p_1|^{-1/4}}\,. \tag{3.51}$$

(Note that p_2 and p_3 commute with the other terms in $\hat{\mathcal{C}}_H^{(4)}$). The operator p_1 is self-adjoint on $\mathcal{H}_{\rm kin}^{\rm grav}$ whence any measurable function of p_1 is also a well-defined self-adjoint operator. However, since kets $|\lambda_1 = 0, \lambda_2, \lambda_3\rangle$ are normalizable in $\mathcal{H}_{\rm kin}^{\rm grav}$, the naïve inverse powers of $\hat{p}_1$ fail to be densely defined and cannot be self-adjoint. To define inverse powers, as is usual in LQG, we will use a variation on the Thiemann inverse triad identities [119, 120]. Classically, we have the identity

$$|p_1|^{-1/4} = -\frac{i\,{\rm sgn}(p_1)}{2\pi G\gamma}\sqrt{\frac{|p_2p_3|}{\Delta\ell_{\rm Pl}^2}}\;e^{-i\bar{\mu}_1 c_1}\,\{e^{i\bar{\mu}_1 c_1}, |p_1|^{1/4}\}\,, \tag{3.52}$$

which holds for any choice of $\bar{\mu}_1$. Since it is most natural to use the same $\bar{\mu}_1$ that featured in the definition of the connection operator, we will make this choice. Eq. (3.52) suggests a natural quantization strategy for $|p_1|^{-1/4}$. Using it and the parity considerations, we are led to the following factor ordering[4]:

$$\widehat{|p_1|^{-1/4}} = -\frac{i\,\mathrm{sgn}(p_1)}{2\pi G\gamma}\sqrt{\frac{|p_2p_3|}{\Delta\ell_{\mathrm{Pl}}^2}}\; e^{-i\bar{\mu}_1c_1/2}\;\frac{1}{i\hbar}[e^{i\bar{\mu}_1c_1}, |p_1|^{1/4}]\; e^{-i\bar{\mu}_1c_1/2}\,, \tag{3.53}$$

where, as is common in LQC, $\mathrm{sgn}(p_1)$ is defined as

$$\mathrm{sgn}(p_1) = \begin{cases} +1 \text{ if } p_1 > 0, \\ \;0 \text{ if } p_1 = 0, \\ -1 \text{ if } p_1 < 0. \end{cases} \tag{3.54}$$

At first it may seem surprising that the expression of $\widehat{|p_1|^{-1/4}}$ involves operators other than p_1. It is therefore important to verify that it has the standard desirable properties. First, as one would hope, it is indeed diagonal in the eigenbasis of the operators $\hat{p}_k$:

$$\widehat{|p_1|^{-1/4}}\,|\lambda_1,\lambda_2,\lambda_3\rangle = \frac{\sqrt{2}\mathrm{sgn}(\lambda_1)\,\sqrt{|\lambda_2\lambda_3|}}{(4\pi\gamma\sqrt{\Delta}\ell_{\mathrm{Pl}}^3)^{1/6}}\cdot\Bigg[\sqrt{|v+\mathrm{sgn}(\lambda_2\lambda_3)|} - \sqrt{|v-\mathrm{sgn}(\lambda_2\lambda_3)|}\Bigg]\,|\lambda_1,\lambda_2,\lambda_3\rangle. \tag{3.55}$$

Second, on eigenkets with large volume, the eigenvalue is indeed well-approximated by $p_1^{-1/4}$, whence on semi-classical states it behaves as the inverse of $\hat{p}^{1/4}$, just as one would hope. Thus, Eq. (3.55) provides a viable candidate for $\widehat{|p_1|^{-1/4}}$. But there are interesting nontrivialities in the Planck regime. In particular, although counter-intuitive, as is common in LQC the operator annihilates states $|\lambda_1,\lambda_2,\lambda_3\rangle$ with $v = 2\lambda_1\lambda_2\lambda_3 = 0$

Finally, note that the operator $\hat{\varepsilon}$ appearing in the expression (3.51) of $\hat{\mathcal{C}}_H^{(4)}$ either operates immediately before or after $\widehat{|p_1|^{-1/4}}$. Since $\widehat{|p_1|^{-1/4}}$ annihilates all zero volume states and $\hat{\varepsilon}$ acts on such states as the identity operator, we only need to consider the action of $\hat{\varepsilon}$ on states with nonzero volume. In this case, $\hat{\varepsilon}$ acts as

[4]In the classical theory, $(L_2L_3)^{1/4}\,|p_1|^{-1/4}$ is independent of the choice of the elementary cell. As pointed out in [48] the inverse triad operators, by contrast, depend on the choice of the cell. However, one can verify that as we remove the regulator, i.e., take the limit $\mathcal{V}\to\mathbb{R}^3$, as in the classical theory, the expression $(L_2L_3)^{1/4}\,\widehat{|p_1|^{-1/4}}$ has a well-defined limit.

$\text{sgn}(v)$. Therefore the action of $\hat{\mathcal{C}}_H^{(4)}$ can be written as:

$$\left[\hat{\mathcal{C}}_H^{(4)}\,\Psi\right](\lambda_1,\lambda_2,\lambda_3) = -\frac{i\alpha\pi\sqrt{\Delta}\hbar\ell_{\text{Pl}}^2}{(4\pi\gamma\sqrt{\Delta})^{1/3}}\ \text{sgn}(v)\ (\lambda_2\lambda_3)^4\cdot\left[\sqrt{|v+\text{sgn}(\lambda_2\lambda_3)|}\right.$$
$$\left. - \sqrt{|v-\text{sgn}(\lambda_2\lambda_3)|}\right]\cdot\left[\Phi^+(\lambda_1,\lambda_2,\lambda_3)-\Phi^-(\lambda_1,\lambda_2,\lambda_3)\right], \quad (3.56)$$

where

$$\Phi^\pm(\lambda_1,\lambda_2,\lambda_3) = \left(\sqrt{|v+\text{sgn}(\lambda_2\lambda_3)(1\pm 2)|}-\sqrt{|v-\text{sgn}(\lambda_2\lambda_3)(1\mp 2)|}\right)$$
$$\times\left[\text{sgn}(v)+\text{sgn}(v\pm 2\text{sgn}(\lambda_2\lambda_3))\right]\Psi(\tfrac{v\pm 2\text{sgn}(\lambda_2\lambda_3)}{v}\cdot\lambda_1,\lambda_2,\lambda_3). \quad (3.57)$$

Recall that in the classical theory the singularity corresponds precisely to the phase space points at which the volume vanishes. Therefore, as in the Bianchi I model, states with support only on points with $v=0$ will be called 'singular' and those which vanish at points with $v=0$ will be called regular. The total Hilbert space $\mathcal{H}_{\text{kin}}^{\text{grav}}$ is naturally decomposed as a direct sum $\mathcal{H}_{\text{kin}}^{\text{grav}}=\mathcal{H}_{\text{sing}}^{\text{grav}}\oplus\mathcal{H}_{\text{reg}}^{\text{grav}}$ of singular and regular subspaces. We will conclude this discussion by examining the action of $\hat{\mathcal{C}}_H^{(4)}$ on these subspaces. Note first that in the action of $\hat{\mathcal{C}}_H^{(4)}$, the state is first acted upon by the operator $\widehat{|p_1|^{-1/4}}$. Since this operator annihilates states $|\lambda_1\lambda_2,\lambda_3\rangle$ with $v=2\lambda_1\lambda_2\lambda_3=0$, singular states are simply annihilated by $\hat{\mathcal{C}}_H^{(4)}$. In particular this implies that the singular subspace is mapped to itself under this action. It is clear from Eq. (3.57) that if Ψ is regular, i.e., Ψ vanishes on all points with $v=0$, $\Phi^\pm$ also vanish at these points. Thus the regular subspace is also preserved by this action. This fact will be used in the discussion of singularity resolution in Sec. 3.3.3.4.

Remark: Our definition of the operator $\widehat{|p|^{-1/4}}$ is not unique; as is common with nontrivial functions of elementary variables, there are factor ordering ambiguities. For example, for $0<n<1/2$, we have the classical identity

$$|p_1|^{n-1/2} = \frac{-i\text{sgn}(p_1)\sqrt{|p_2p_3|}}{8\pi\gamma\sqrt{\Delta}G\ell_{\text{Pl}}n}e^{-i\bar{\mu}_1c_1}\left\{e^{i\bar{\mu}_1c_1},|p_1|^n\right\}\ .$$

Hence, it is possible to instead define $\widehat{p_1^{-1/4}}$ as

$$\widehat{p_1^{-1/4}} = \left(\widehat{|p_1|^{n-1/2}}\right)^{-1/(4n-2)}$$

where

$$\widehat{|p_1|^{n-1/2}} = -\frac{(4\pi\gamma\sqrt{\Delta}\ell_{\mathrm{Pl}}^3)^{(2+2n)/3}}{4^n(8\pi\gamma G\sqrt{\Delta}\ell_{\mathrm{Pl}})^3 n}\mathrm{sgn}(\lambda_1)|\lambda_2\lambda_3|^{1-2n} \times \Big[|v+\mathrm{sgn}(\lambda_2\lambda_3)|^{2n} - |v-\mathrm{sgn}(\lambda_2\lambda_3)|^{2n}\Big].$$

For $n \neq \frac{1}{4}$, this choice for the operator $\widehat{p_1^{-1/4}}$ is not equivalent to the one we chose. These two choices are both well-defined and admit the same classical limit but they differ in the Planck regime. It is also possible to construct other such inequivalent $\widehat{p_1^{-1/4}}$ candidate operators. For definiteness we have made the 'simplest' choice.

3.3.3.3 The Fifth Term in $\hat{\mathcal{C}}_H$

Let us now consider the last term in the expression of the gravitational part of the Hamiltonian constraint,

$$\hat{\mathcal{C}}_H^{(5)} = \frac{\alpha^2}{32\pi G\gamma^2}(1+\gamma^2)\,(p_2p_3)^2\;\widehat{p_1^{-2}}. \tag{3.58}$$

This term is simpler since it only involves powers of p_k and we are working in a representation where p_k are diagonal. From our discussion of the last section, it is natural to set

$$\widehat{p_1^{-2}} := \left(\widehat{p_1^{-1/4}}\right)^8, \tag{3.59}$$

then we have

$$\hat{\mathcal{C}}_H^{(5)}\,\Psi(\lambda_1,\lambda_2,\lambda_3) = \frac{8\pi\alpha^2\Delta(1+\gamma^2)\hbar\ell_{\mathrm{Pl}}^2}{(4\pi\gamma\sqrt{\Delta})^{2/3}}\,\mathrm{sgn}(\lambda_1)^8\lambda_2^8\lambda_3^8 \times\left(\sqrt{|v+\mathrm{sgn}(\lambda_2\lambda_3)|}-\sqrt{|v-\mathrm{sgn}(\lambda_2\lambda_3)|}\right)^8\Psi(\lambda_1,\lambda_2,\lambda_3). \tag{3.60}$$

Again, it is clear that if $v=0$, the wave function is annihilated by this part of the constraint. Also, it follows by inspection that the singular and regular subspaces are both mapped to themselves by the action of $\hat{\mathcal{C}}_H^{(5)}$.

3.3.3.4 Singularity Resolution

We can now determine the gravitational part $\hat{\mathcal{C}}_{\rm grav}$ of the Hamiltonian constraint by combining the results of Chapter 2 and Eqs. (3.56) and (3.60). We have:

$$\hat{\mathcal{C}}_{\rm grav} = \hat{\mathcal{C}}_{\rm grav}^{\rm (BI)} + \hat{\mathcal{C}}_H^{(4)} + \hat{\mathcal{C}}_H^{(5)}, \tag{3.61}$$

where $\hat{\mathcal{C}}_{\rm grav}^{\rm (BI)}$ is the gravitational part of the Hamiltonian constraint in the Bianchi I model [86]. There is however a conceptual subtlety. In the classical theory the Hamiltonian density $\mathcal{C}_{\rm grav}/(L_1L_2L_3)^2$ is independent of the choice of the elementary cell [where we have to divide by $(L_1L_2L_3)^2$ because the lapse corresponding to harmonic time scales as $(L_1L_2L_3)$ and the Hamiltonian constraint is obtained by integration over the elementary cell $\mathcal{V}$]. As shown in Sec. 2.5, $\hat{\mathcal{C}}_{\rm grav}^{\rm (BI)}/(L_1L_2L_3)^2$ is again independent of the choice of the elementary cell $\mathcal{V}$. However, the two additional terms that are special to the Bianchi II model are not independent of $\mathcal{V}$ because they involve the inverse-triad operators [48]. Nonetheless, in the limit as we take the regulator away, i.e., $\mathcal{V} \to \mathbb{R}^3$, the operator $\hat{\mathcal{C}}_{\rm grav}/(L_1L_2L_3)^2$ has a well-defined limit (see footnote 5). Strictly speaking, in the discussion of Bianchi II quantum dynamics, we have to work with this limit, rather than with operators defined using a fixed cell.

As in the Bianchi I model, the action simplifies if we replace one of the λ_i by v. In the Bianchi I model, it does not matter which of the λ_i is replaced because of the additional symmetry of that model. In the Bianchi II case, while it remains possible to replace any of the λ_i, it is simplest to replace λ_1 by v and represent quantum states as $\Psi = \Psi(\lambda_2, \lambda_3, v; T)$. This change of variables would be nontrivial if, as in the Wheeler-DeWitt theory, we had used the Lesbegue measure in the gravitational sector. However, it is quite tame here because the norms are defined using a discrete measure. The inner product on $\mathcal{H}_{\rm kin}^{\rm grav}$ is now given by

$$\langle \Psi_1 | \Psi_2 \rangle_{\rm kin} = \sum_{\lambda_2, \lambda_3, v} \bar{\Psi}_1(\lambda_2, \lambda_3, v)\, \Psi_2(\lambda_2, \lambda_3, v) \tag{3.62}$$

and states are symmetric under the action of $\hat{\Pi}_k$. In Appendix A, we show that, under the action of reflections $\hat{\Pi}_i$, the operators $\sin \bar{\mu}_i c_i$ have the same transformation properties that c_i have under reflections Π_i in the classical theory. As a consequence, $\hat{\mathcal{C}}_{\rm grav}$ is also reflection symmetric. Therefore, its action is well-defined on $\mathcal{H}_{\rm kin}^{\rm grav}$: $\hat{\mathcal{C}}_{\rm grav}$ is a densely defined, symmetric operator on this Hilbert space. In the isotropic case, its analog has been shown to be essentially self-adjoint [40]. In what follows we will assume that $\hat{\mathcal{C}}_{\rm grav}$ is essentially self-adjoint on $\mathcal{H}_{\rm kin}^{\rm grav}$ and work with its self-adjoint extension.

It is now straightforward to write down the full Hamiltonian constraint on $\mathcal{H}_{\rm kin}^{\rm grav}$:

$$-\hbar^2\, \partial_T^2\, \Psi(\lambda_2, \lambda_3, v; T) = \hat{\Theta}\, \Psi(\lambda_2, \lambda_3, v; T), \quad \text{where} \quad \hat{\Theta} = -2\hat{\mathcal{C}}_{\rm grav}. \tag{3.63}$$

As in the isotropic case [33], one can obtain the physical Hilbert space $\mathcal{H}_{\rm phy}$ by a group averaging procedure and the final result is completely analogous. Elements of $\mathcal{H}_{\rm phy}$ consist of 'positive frequency' solutions to Eq. (3.63), i.e., solutions to

$$-i\hbar\partial_T \Psi(\lambda_2, \lambda_3, v; T) \;=\; \sqrt{|\hat{\Theta}|}\, \Psi(\lambda_2, \lambda_3, v; T)\,, \tag{3.64}$$

which are symmetric under the three reflection maps $\hat{\Pi}_i$, i.e., satisfy

$$\Psi(\lambda_2, \lambda_3, v;\, T) = \Psi(|\lambda_2|, |\lambda_3|, |v|;\, T)\,. \tag{3.65}$$

The scalar product is given simply by

$$\begin{aligned} \langle \Psi_1 | \Psi_2 \rangle_{\rm phys} &= \langle \Psi_1(\lambda_2, \lambda_3, v; T_o) | \Psi_2(\lambda_2, \lambda_3, v; T_o) \rangle_{\rm kin} \\ &= \sum_{\lambda_1, \lambda_2, \lambda_3} \bar{\Psi}_1(\vec{\lambda}, T_o)\, \Psi_2(\vec{\lambda}, T_o), \end{aligned} \tag{3.66}$$

where T_o is any "instant" of internal time T.

We can now address the issue of singularity resolution using general properties of various operators. Recall that the gravitational part of the Hamiltonian constraint operator in the Bianchi I model shares two properties with the fourth and the fifth terms studied above which are specific to the Bianchi II model. First, it annihilates singular states and, second, singular states decouple from the regular states under its action. Therefore the full Bianchi II Hamiltonian constraint also has these two properties. Since the singular states decouple from regular states[5], an initial state in the regular subspace cannot become singular during evolution. It is in this precise sense that the classical singularity is resolved. Sometimes one considers weaker forms of singularity resolution. For example, it could happen that the evolution of the wave function is always well-defined but a regular state can evolve to the singular subspace. For the Bianchi I and II models, the singularity is resolved in a stronger sense: *Not only is the evolution well-defined at all times, but the singular states (are stationary and) decouple entirely from the regular ones.*

3.3.3.5 The Explicit Form of the Hamiltonian Constraint

We will conclude by providing an explicit form of the full quantum constraint equation that will be needed in numerical simulations.

Recall that in the Bianchi I model symmetries enabled us to restrict our attention to the positive octant of the 3-dimensional space spanned by $(\lambda_1, \lambda_2, \lambda_3)$. This is again the case for the Bianchi II model. More precisely, elements of $\mathcal{H}_{\rm kin}^{\rm grav}$ are invariant under the three parity maps $\hat{\Pi}_k$ and, as shown in Appendix A, the Hamiltonian constraint satisfies $\hat{\Pi}_k \hat{\mathcal{C}}_{\rm grav} \hat{\Pi}_k = \hat{\mathcal{C}}_{\rm grav}$. Therefore, knowledge of the restriction of the image $\hat{\mathcal{C}}_{\rm grav}\Psi$ of Ψ to the positive octant suffices to determine $\hat{\mathcal{C}}_{\rm grav}\Psi$ completely. In the positive octant, $\mathrm{sgn}(\lambda_k)$ can only be 0 or 1 which simplifies the action of operators. Therefore, in the remainder of this section we will restrict the argument of $\hat{\mathcal{C}}_H\Psi$ to the positive octant. The full action is given simply by

$$\big(\hat{\mathcal{C}}_{\rm grav}\Psi\big)(\lambda_2, \lambda_3, v) = \big(\hat{\mathcal{C}}_{\rm grav}\Psi\big)(|\lambda_2|, |\lambda_3|, |v|). \tag{3.67}$$

Since the singular states are annihilated by $\hat{\mathcal{C}}_{\rm grav}$, their evolution is trivial:

$$\partial_T^2\, \Psi(\lambda_2, \lambda_3, v = 0; T) = 0\,. \tag{3.68}$$

Nonsingular states are physically more relevant. On them, the explicit form of the

[5] Singular states are in the kernel of Θ and regular states are orthogonal to the singular ones. From spectral decomposition one expects $\sqrt{\Theta}$ to have the same property. However, to complete this argument, one would have to establish that $\hat{\mathcal{C}}_{\rm grav}$ is essentially self-adjoint and its self adjoint extension also shares this property.

full constraint is given by:

$$\begin{aligned}\partial_T^2\,\Psi = \frac{\pi G}{8}\Bigg[&\sqrt{v}\Big((v+2)\sqrt{v+4}\,\Psi_4^+ - (v+2)\sqrt{v}\,\Psi_0^+ \\ &- \theta_{v-2}(v-2)\sqrt{v}\,\Psi_0^- + \theta_{v-4}(v-2)\sqrt{|v-4|}\,\Psi_4^-\Big) \\ &+ \frac{8i\alpha\sqrt{\Delta}}{(4\pi\gamma\sqrt{\Delta})^{1/3}} \times (\lambda_2\lambda_3)^4\left(\sqrt{v+1}-\sqrt{|v-1|}\right)\left(\Phi^- - \Phi^+\right) \\ &+ \frac{64\alpha^2\Delta(1+\gamma^2)}{(4\pi\gamma\sqrt{\Delta})^{2/3}}(\lambda_2\lambda_3)^8\,(\sqrt{v+1}-\sqrt{|v-1|})^8\,\Psi\Bigg], \end{aligned} \tag{3.69}$$

we have dropped the arguments of the Ψ and Φ's to simplify the notation, the argument is $(\lambda_2, \lambda_3, v; T)$ in each case. The $\Psi^{\pm}_{0,4}$ are defined as follows:

$$\begin{aligned}\Psi^{\pm}_n(\lambda_2,\lambda_3,v;T) = {}&\Psi\left(\tfrac{v\pm n}{v\pm 2}\cdot\lambda_2, \tfrac{v\pm 2}{v}\cdot\lambda_3, v\pm n; T\right) + \Psi\left(\tfrac{v\pm n}{v\pm 2}\cdot\lambda_2, \lambda_3, v\pm n; T\right) \\ &+ \Psi\left(\tfrac{v\pm 2}{v}\cdot\lambda_2, \tfrac{v\pm n}{v\pm 2}\cdot\lambda_3, v\pm n; T\right) + \Psi\left(\tfrac{v\pm 2}{v}\cdot\lambda_2, \lambda_3, v\pm n; T\right) \\ &+ \Psi\left(\lambda_2, \tfrac{v\pm 2}{v}\cdot\lambda_3, v\pm n; T\right) + \Psi\left(\lambda_2, \tfrac{v\pm n}{v\pm 2}\cdot\lambda_3, v\pm n; T\right), \end{aligned} \tag{3.70}$$

while $(\Phi^- - \Phi^+)$ is given by

$$\begin{aligned}\big(\Phi^- - \Phi^+\big)(\lambda_2,\lambda_3,v;T) = {}&2\theta_{v-2}(\sqrt{|v-1|}-\sqrt{|v-3|})\cdot\Psi(\lambda_2,\lambda_3,v-2;T)\Big] \\ &- 2(\sqrt{v+3}-\sqrt{v+1})\cdot\Psi(\lambda_2,\lambda_3,v+2;T). \end{aligned} \tag{3.71}$$

(The imaginary coefficients in Eq. (3.69) come from the action of single $\sin\bar{\mu}_i c_i$ terms.)

Equation (3.69) immediately implies that, as in the Bianchi I model, the steps in v are uniform: the argument of the wave function only involves $v-4, v-2, v, v+2$ and $v+4$. Thus, there is a superselection in v. For each $\epsilon \in [0, 2)$, let us introduce a lattice $\mathcal{L}_\epsilon$ of points $v = 2n+\epsilon$. Then the quantum evolution —and the action of the Dirac observables $\hat{p}_T$ and $\hat{V}|_T$ commonly used in LQC— preserves the subspaces $\mathcal{H}^\epsilon_{\rm phy}$ consisting of states with support in v on $\mathcal{L}_\epsilon$. The most interesting lattice is the one corresponding to $\epsilon = 0$ since it includes the classically singular points $v = 0$.

Finally, it is obvious from Eq. (3.69) that in the limit $\alpha \to 0$ quantum dynamics of the Bianchi II model reduces to that of the Bianchi I model discussed in Chapter 2. In particular, it is possible to obtain the LQC dynamics for the k=0 FLRW cosmology from this model by first taking $\alpha \to 0$ and then following the projection map defined in Sec. 2.4.1.

3.4 Effective Equations

In the isotropic models, effective equations have been introduced via two different approaches —the embedding and the truncation methods. Both start by regarding the space of quantum states as an infinite dimensional symplectic manifold —the quantum phase space— which is also equipped with a Kähler structure that descends from the Hermitian inner product on the Hilbert space. In the first method, one finds a judicious embedding of the classical phase space into the quantum phase space which is approximately preserved by the quantum evolution vector field [37, 38]. By projecting this vector field into the image of the embedding one obtains quantum corrected effective equations. In the isotropic case these effective equations provide an excellent approximation to the full quantum evolution of states which are Gaussians at late times, even in the $\Lambda \neq 0$ as well as k=$\pm$1 cases where the models are not exactly soluble. In the second method one uses expectation values, uncertainties, and higher moments to define a convenient system of coordinates on the infinite dimensional phase space. The exact quantum evolution equations are then a set of coupled nonlinear ordinary differential equations for these coordinates. By a judicious truncation of this system one obtains effective equations containing quantum corrections [121]. In its spirit the first method is analogous to the 'variational principle technique' used in perturbation theory, in that it requires a judicious combination of art (of selecting the embedding) and science. It is often simpler to use and can be surprisingly accurate. The second method is more systematic, similar in our analogy to the standard, order by order perturbation theory. It is also more general in the sense that it is applicable to a wide variety of states. In this section we will use the first method to gain qualitative insights into leading order quantum effects.

To obtain the effective equations, without loss of generality we can restrict our attention to the positive octant of the classical phase space (where $\varepsilon = 1$). Then the quantum corrected Hamiltonian constraint is given by the classical analogue of (3.46):

$$\frac{p_T^2}{2} + \mathcal{C}_{\rm grav}^{\rm eff} = 0, \tag{3.72}$$

where

$$\begin{aligned} \mathcal{C}_{\rm grav}^{\rm eff} = &- \frac{p_1 p_2 p_3}{8\pi G \gamma^2 \Delta \ell_{\rm Pl}^2} \left[\sin \bar\mu_1 c_1 \sin \bar\mu_2 c_2 + \sin \bar\mu_2 c_2 \sin \bar\mu_3 c_3 + \sin \bar\mu_3 c_3 \sin \bar\mu_1 c_1 \right] \\ &- \frac{1}{8\pi G \gamma^2} \left[\frac{\alpha (p_2 p_3)^{3/2}}{\sqrt{\Delta}\ell_{\rm Pl}\sqrt{p_1}} \sin \bar\mu_1 c_1 - (1+\gamma^2)\left(\frac{\alpha p_2 p_3}{2 p_1} \right)^2 \right]. \end{aligned} \tag{3.73}$$

Using the expressions (3.39) for $\bar\mu_k$, it is easy to verify that far away from the classical singularity —more precisely in the regime in which the (gauge fixed) spin connection and the extrinsic curvature are sufficiently small so that $c_k \bar\mu_k \ll 1$— the effective Hamiltonian constraint in Eq. (3.72) is well-approximated by the classical one in Eq. (3.20).

Since $\sin\theta$ is bounded by 1 for all θ, these equations imply that the matter density $\rho_{\rm matt} = p_T^2/2V^2 = p_T^2/2p_1p_2p_3$ satisfies

$$\rho_{\rm matt} \le \frac{3}{8\pi\gamma^2 \Delta G \ell_{\rm Pl}^2} + \frac{1}{8\pi\gamma^2 G}\left[\frac{x}{\sqrt{\Delta}\ell_{\rm Pl}} - \frac{(1+\gamma^2)x^2}{4} \right], \tag{3.74}$$

where we have introduced $x := \alpha\sqrt{p_2 p_3/p_1^3}$. The maximum of the expression in square brackets is attained at $x = 2/(1+\gamma^2)\sqrt{\Delta}\ell_{\rm Pl}$, whence

$$\rho_{\rm matt} \le \frac{3 + (1+\gamma^2)^{-1}}{8\pi\gamma^2\Delta G \ell_{\rm Pl}^2} \approx 0.54 \rho_{\rm Pl}. \tag{3.75}$$

Thus, on the constraint surface in the phase space defined by Eq. (3.72), the matter energy density is bounded by $0.54\rho_{\rm Pl}$. But this bound may be far from being optimal. In all isotropic models, the optimal bound on matter density was found to be $0.41\rho_{\rm Pl}$. In the Bianchi I model, simulations by Vandersloot [113] show that the 'volume bounce' occurs when matter density is *lower* than $0.41\rho_{\rm Pl}$ because there is also energy density in gravitational waves. It would be interesting to use numerical simulations to find out what happens for generic solutions to the

Bianchi II effective equations.

Finally, to obtain the effective equations for each variable, one simply takes its Poisson bracket with the effective Hamiltonian constraint. This gives the effective equations

$$\dot{p_1} = \gamma^{-1}\left(\frac{p_1^2}{\bar{\mu}_1}(\sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_3 c_3) + \alpha p_2 p_3\right)\cos\bar{\mu}_1 c_1, \tag{3.76}$$

$$\dot{p_2} = \frac{p_2^2}{\gamma\bar{\mu}_2}(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_3 c_3)\cos\bar{\mu}_2 c_2, \tag{3.77}$$

$$\dot{p_3} = \frac{p_3^2}{\gamma\bar{\mu}_3}(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_2 c_2)\cos\bar{\mu}_3 c_3, \tag{3.78}$$

$$\begin{aligned}\dot{c_1} = -\frac{1}{\gamma}\Big[&\frac{p_2 p_3}{\Delta\ell_{\rm Pl}^2}\big(\sin\bar{\mu}_1 c_1 \sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_1 c_1 \sin\bar{\mu}_3 c_3 + \sin\bar{\mu}_2 c_2 \sin\bar{\mu}_3 c_3 \\ &+ \frac{\bar{\mu}_1 c_1}{2}\cos\bar{\mu}_1 c_1(\sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_3 c_3) - \frac{\bar{\mu}_2 c_2}{2}\cos\bar{\mu}_2 c_2(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_3 c_3) \\ &- \frac{\bar{\mu}_3 c_3}{2}\cos\bar{\mu}_3 c_3(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_2 c_2)\big) + (1+\gamma^2)\alpha^2\frac{(p_2 p_3)^2}{2p_1^3} \\ &+ \frac{\alpha}{2\sqrt{\Delta}\ell_{\rm Pl}}\left(\frac{p_2 p_3}{p_1}\right)^{3/2}(\bar{\mu}_1 c_1 \cos\bar{\mu}_1 c_1 - \sin\bar{\mu}_1 c_1)\Big],\end{aligned} \tag{3.79}$$

$$\begin{aligned}\dot{c_2} = -\frac{1}{\gamma}\Big[&\frac{p_1 p_3}{\Delta\ell_{\rm Pl}^2}\big(\sin\bar{\mu}_1 c_1 \sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_1 c_1 \sin\bar{\mu}_3 c_3 + \sin\bar{\mu}_2 c_2 \sin\bar{\mu}_3 c_3 \\ &- \frac{\bar{\mu}_1 c_1}{2}\cos\bar{\mu}_1 c_1(\sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_3 c_3) + \frac{\bar{\mu}_2 c_2}{2}\cos\bar{\mu}_2 c_2(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_3 c_3) \\ &- \frac{\bar{\mu}_3 c_3}{2}\cos\bar{\mu}_3 c_3(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_2 c_2)\big) - (1+\gamma^2)\alpha^2\frac{p_2 p_3^2}{2p_1^2} \\ &+ \frac{\alpha p_3}{2\bar{\mu}_1}(3\sin\bar{\mu}_1 c_1 - \bar{\mu}_1 c_1 \cos\bar{\mu}_1 c_1)\Big],\end{aligned} \tag{3.80}$$

$$\begin{aligned}\dot{c_3} = -\frac{1}{\gamma}\Big[&\frac{p_1 p_2}{\Delta\ell_{\rm Pl}^2}\big(\sin\bar{\mu}_1 c_1 \sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_1 c_1 \sin\bar{\mu}_3 c_3 + \sin\bar{\mu}_2 c_2 \sin\bar{\mu}_3 c_3 \\ &- \frac{\bar{\mu}_1 c_1}{2}\cos\bar{\mu}_1 c_1(\sin\bar{\mu}_2 c_2 + \sin\bar{\mu}_3 c_3) - \frac{\bar{\mu}_2 c_2}{2}\cos\bar{\mu}_2 c_2(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_3 c_3) \\ &+ \frac{\bar{\mu}_3 c_3}{2}\cos\bar{\mu}_3 c_3(\sin\bar{\mu}_1 c_1 + \sin\bar{\mu}_2 c_2)\big) - (1+\gamma^2)\alpha^2\frac{p_2^2 p_3}{2p_1^2} \\ &+ \frac{\alpha p_2}{2\bar{\mu}_1}(3\sin\bar{\mu}_1 c_1 - \bar{\mu}_1 c_1 \cos\bar{\mu}_1 c_1)\Big].\end{aligned} \tag{3.81}$$

In the “embedding approach” these effective equations provide the leading-order quantum corrections to the classical equations of motion Eqs. (3.23)–(3.28). It would be very interesting to numerically test if the accuracy they display in the isotropic case for states which are Gaussians at late times carries over to the Bianchi II case.

3.5 Discussion

In this chapter, we analyzed the “improved” LQC dynamics of the Bianchi II model. As in the isotropic and Bianchi I cases, we chose the matter source to be a massless scalar field since it can to serve as a viable relational time parameter in both the classical and the quantum theories. It is again rather straightforward to accommodate additional matter fields in this framework.

Our broad strategy is the same as that used in the Bianchi I model. However, because Bianchi II models have anisotropies as well as spatial curvature, holonomies around closed curves are no longer guaranteed to be almost periodic functions of the connection. Hence, one cannot use them to construct the field strength operator on the LQC Hilbert space; a new conceptual and technical input is necessary to define the quantum Hamiltonian constraint operator. We overcame this difficulty by generalizing the strategy used so far [31, 34, 43, 46, 47, 48, 49, 86]. Specifically, we used holonomies around open segments parallel to the fiducial triads $\mathring{e}^a_i$ to define a connection operator. This strategy is also inspired by methods introduced by Thiemann in the full theory [119, 120]. However, because of gauge fixing LQC does not enjoy the manifest diffeomorphism invariance of full LQG. As a consequence, in LQC one needs a principle to fix the ‘length’ of the open segment along which holonomy is evaluated. We required that the ‘length’ be so chosen that the field strength operator constructed from the resulting connection should agree with that constructed from holonomies around closed loops whenever the second construction is available. This guarantees that (apart from ‘tame’ factor ordering ambiguities) the new procedure reduces to the one used in the LQC literature before. Moreover, the strategy of defining the Hamiltonian constraint through this connection operator can be used also in more general contexts. In particular, it enables one to overcome a conceptual limitation of the otherwise complete treatment of the isotropic, k=-1 model given in [48, 49]. More importantly, it extends to more general class A Bianchi models.

There is a second —but primarily technical— difference from the Bianchi I case: the Hamiltonian operator now contains inverse powers of p_1. This was handled following a general method introduced by Thiemann to define inverse triad operators in LQG [119, 120]. As usual, there is a factor ordering ambiguity. In the main discussion we used the simplest operator which has the same symmetries with respect to parity as its classical counterpart.

After addressing these two issues, we obtained a well-defined quantum Hamiltonian constraint and showed that the singularity in Bianchi II models is resolved in the same precise sense as in the FLRW and Bianchi I models. The kinematical Hilbert space $\mathcal{H}_{\rm kin}^{\rm grav}$ can be decomposed as $\mathcal{H}_{\rm kin}^{\rm grav} = \mathcal{H}_{\rm sing}^{\rm grav} \oplus \mathcal{H}_{\rm reg}^{\rm grav}$ where states in the singular subspace have support only on configurations with zero volume, while those in the regular subspace have no support on these singular configurations. *The Hamiltonian constraint operator annihilates states in* $\mathcal{H}_{\rm sing}^{\rm grav}$ *and maps* $\mathcal{H}_{\rm reg}^{\rm grav}$ *to itself.* We also provided an explicit form of the action of the Hamiltonian constraint operator which should be helpful in performing numerical simulations.

Finally, we obtained effective equations using the "embedding method" introduced by Willis [37] and further developed by Taveras [38] in the isotropic case. There, although the assumptions made in the derivation fail in the deep Planck regime, the final equations provide a surprisingly accurate approximation to the full quantum evolution of states which are Gaussians at late times. This holds not only for the exactly soluble k=0, $\Lambda = 0$ model but also for the much more complicated $\Lambda \neq 0$ and k=± 1 models. It would be interesting to see if this phenomenon extends also to Bianchi II models. Furthermore, numerical solutions of these effective equations themselves may be of considerable interest because the simplest upper bound on matter density they lead to is higher than that in all other models studied so far, including Bianchi I. Numerical simulations of effective equations will answer several questions within this approximation. Is the upper bound optimal, i.e., do generic solutions to effective equations come close to saturating it? In the Bianchi I case, numerical simulations by Vandersloot [113] revealed that, unlike in the isotropic model, there are several distinct kinds of 'bounces.' Roughly, anytime a shear —or a Weyl curvature— scalar enters the Planck regime, quantum geometry repulsion comes into pay in a dominant manner and 'dilutes' that scalar, preventing a blow up. How do additional terms in the Bianchi II effective equations affect this scenario? Qualitative lessons from numerical simulations would be valuable in developing further intuition for various quantum geometry effects.

Chapter 4

Bianchi Type IX Models

4.1 Introduction

At the classical level, the Bianchi IX model has a much richer phenomenology than Bianchi I and II models as it displays Mixmaster dynamics as the singularity is approached [92]. In essence, a space-time which exhibits Mixmaster dynamics is one which can be described for long periods of time (known as epochs) as a Bianchi I space-time characterized by three anisotropic expansion rates. Such a space-time will occasionally undergo a "Mixmaster bounce" from one epoch to another where the three expansion rates change in a specific manner. Bianchi I models approach the singularity in a rather straightforward way as they do not undergo any Mixmaster bounces while Bianchi II models may undergo a single Mixmaster bounce between two epochs as the singularity is approached (see [92] and references therein). The Bianchi IX model, on the other hand, undergoes many Mixmaster bounces and this behaviour is chaotic [92, 122]. Since much of this behaviour occurs when the curvature is near (or beyond) the Planck scale, quantum gravity effects cannot be neglected and the Mixmaster behaviour may be significantly modified when they are taken into account.

Bianchi IX models are also thought to play an important role near generic singularities in classical general relativity. The Belinskii, Khalatnikov, Lifshitz (BKL) conjecture suggests that as a generic space-like singularity is approached, time derivatives dominate over spatial derivatives whence physical fields at each point evolve independently from those at neighbouring points. Dynamics can therefore be approximated by the ODE's used in homogeneous space-times, most generally a Bianchi IX solution with a massless scalar field [71, 72]. Since other matter fields do not contribute significantly to the dynamics as the singularity is approached, we will only consider the case of a massless scalar field in this work. There has recently been a considerable amount of numerical work supporting this paradigm (see, e.g., [92]) and the conjecture has also been rewritten in terms of variables suitable to a loop quantization [99]. If the BKL conjecture is indeed correct, it follows that a good understanding of the quantum dynamics of the Bianchi IX model in the deep quantum regime could lead to major insights into the behaviour of *generic* space-times in regions where the curvature reaches the Planck scale.

Because of the Bianchi IX model's importance, it has already been the subject of studies within the framework of loop quantum cosmology, both in a pre-μ_o-type Hamiltonian framework [74, 75, 76] and in a spin-foam-inspired dipole cosmology model (first introduced for the isotropic case in [66]) which also allows inhomogeneities [67]. However, it is important to study the improved $\bar{\mu}_i$-type dynamics of LQC since the predictions of the pre-μ_o approach are unphysical in the infrared limit. In particular, in isotropic cosmological models quantum gravity effects can become important at energy densities arbitrarily below the Planck scale in this scheme. To ensure that quantum gravity effects only become important at the Planck scale, one must instead use the improved dynamics approach in the Hamiltonian framework[1]. On the other hand, since the dipole cosmology model presented in [67] is inspired by spin foam models, that approach is complementary to ours and it will be interesting to compare the results of these two frameworks.

As pointed out above, chaotic behaviour appears as the singularity is approached in classical Bianchi IX space-times. It has been argued in the pre-μ_o LQC treatment of the model that this behaviour is avoided in LQC due to quantum gravity effects [75, 76]. In essence, the argument is that quantum gravity effects become important before a significant number of Mixmaster bounces occur. Since the quantum gravity effects are repulsive, the space-time will exit the Planck regime having only undergone a small number of Mixmaster bounces and hence the dynamics are not chaotic. In this chapter, we see that in some cases this occurs

[1]It is possible that once the curvature reaches the Planck scale a scheme other than $\bar{\mu}_i$ may be the correct one but we will only consider the $\bar{\mu}_i$ scheme here.

already in the effective theory which incorporates quantum geometry effects into the dynamics. However, we cannot yet show that this is a generic result. We will go into more detail in Sec. 4.4.

The outline of this chapter is as follows. In Sec. 4.2, we will briefly review the necessary classical properties of the Bianchi type IX model in order to proceed with the quantization. In Sec. 4.3 we will study the quantum properties of the model, first recalling the kinematics which are the same as for the Bianchi type I and type II models studied in Chapters 2 and 3. We will then study the Hamiltonian constraint operator for the Bianchi IX model with a massless scalar field as the matter field. The Hamiltonian constraint operator gives an evolution equation where the scalar field acts as a relational time parameter. The dynamics of the model are obtained by using the same technology that was developed during the study of the improved LQC dynamics of the Bianchi type I and type II models; *there is no need to introduce any new operators.* In Sec. 4.4 we will derive effective equations which include modifications to the classical equations of motion due to quantum geometry effects and in Sec. 4.5 we summarize our results and discuss open issues.

4.2 Classical Theory

In Bianchi models [104, 117, 118], one restricts oneself to those phase space variables which admit a 3-dimensional group of symmetries which act simply and transitively. This indicates that Bianchi space-times are homogeneous but not (necessarily) isotropic. In this sense, Bianchi cosmologies can be seen as a natural generalization of FLRW models which allow anisotropic degrees of freedom.

The symmetries allowed in the Bianchi IX group are the three spatial rotations on S^3. It follows that the three Killing (left invariant) vector fields $\mathring{\xi}_i^a$ satisfy[2]

$$[\mathring{\xi}_i,\, \mathring{\xi}_j] = \frac{2}{r_o}\mathring{\epsilon}^k{}_{ij}\mathring{\xi}_k, \tag{4.1}$$

where the structure constants are given by the completely antisymmetric tensor

[2]Here we are following the convenctions used in [67]. A different, although equivalent, choice is used in [46, 74, 75, 76] where the structure constants differ by an overall sign.

$\mathring{\epsilon}_{ijk}$ times $2/r_o$ where r_o is the radius of the 3-sphere with respect to the fiducial metric. $\mathring{\epsilon}_{ijk}$ is defined such that $\mathring{\epsilon}_{123} = 1$, note that the internal indices $i, j, k, \ldots$ can always be freely raised and lowered. There is also a canonical triad $\mathring{e}_i^a$ —the right invariant vector fields— which is Lie dragged by $\mathring{\xi}_i^a$. It is convenient to use $\mathring{e}_i^a$ and its dual co-triad $\mathring{\omega}_a^i$ as fiducial frames and co-frames. They satisfy:

$$[\mathring{e}_i,\, \mathring{e}_j] = -\frac{2}{r_o}\mathring{\epsilon}^k{}_{ij}\, \mathring{e}_k, \qquad \mathrm{d}\,\mathring{\omega}^k = \frac{1}{r_o}\,\mathring{\epsilon}^k{}_{ij}\mathring{\omega}^i \wedge \mathring{\omega}^j. \tag{4.2}$$

The form of the equations above indicates that M admits global coordinates $\alpha \in [0, 2\pi), \beta \in [0, \pi)$ and $\gamma \in [0, 4\pi)$ such that for $r_o = 2$ the Bianchi IX co-triads have the form

$$\begin{aligned} \mathring{\omega}_a^1 &= \sin\beta \sin\gamma(\mathrm{d}\alpha)_a + \cos\gamma(\mathrm{d}\beta)_a, \\ \mathring{\omega}_a^2 &= -\sin\beta\cos\gamma(\mathrm{d}\alpha)_a + \sin\gamma(\mathrm{d}\beta)_a, \\ \mathring{\omega}_a^3 &= \cos\beta(\mathrm{d}\alpha)_a + (\mathrm{d}\gamma). \end{aligned} \tag{4.3}$$

The fiducial co-triads determine a fiducial 3-metric $\mathring{q}_{ab} := \mathring{\omega}_a^i \mathring{\omega}_{bi}$,

$$\mathring{q}_{ab}\mathrm{d}x^a\mathrm{d}x^b = \mathrm{d}\alpha^2 \,+\, \mathrm{d}\beta^2 \,+\, \mathrm{d}\gamma^2 \,+\, 2\cos\beta\mathrm{d}\alpha\mathrm{d}\gamma. \tag{4.4}$$

It follows that $\sqrt{\mathring{q}} = \sin\beta$ and one can see that $\mathring{q}_{ab}$ is the metric of a 3-sphere with a volume $V_o = 16\pi^2$, this agrees with $V_o = 2\pi^2 r_o^3$ for $r_o = 2$ as specified above. Finally, we introduce the length-scale $\ell_o = V_o^{1/3}$ for later convenience.

In diagonal Bianchi models, the physical triads e_i^a are related to the fiducial ones by[3]

$$\omega_a^i = a^i(\tau)\mathring{\omega}_a^i \qquad \text{and} \qquad a_i(\tau)e_i^a = \mathring{e}_i^a, \tag{4.5}$$

where the a_i are the three directional scale factors. Note that if the three scale factors (and their time derivatives) are equal, the metric given by the co-triads is that of a closed isotropic FLRW space-time.

For later use, let us calculate the spin connection determined by the physical

[3]As usual, there is no sum if repeated indices are both covariant or contravariant. The Einstein summation convention holds if a covariant index is contracted with a contravariant index.

triads e^a_i. Since Γ^i_a is given by

$$\Gamma^i_a = -\epsilon^{ijk}\, e^b_j \left(\partial_{[a}\omega_{b]k} + \frac{1}{2} e^c_k \omega^l_a \partial_{[c}\omega_{b]l}\right) , \tag{4.6}$$

it follows that

$$\Gamma^1_a = \frac{\varepsilon}{r_o}\left(\frac{a_1^2}{a_2 a_3} - \frac{a_2}{a_3} - \frac{a_3}{a_2}\right) \mathring{\omega}^1_a, \tag{4.7}$$

where $\varepsilon := \epsilon_{123}$ is $+1$ for right-handed physical triads and -1 for left-handed physical triads. Note that while the $\mathring{\epsilon}_{ijk}$ appearing in the Bianchi IX structure constants are *not* affected by the handedness of the physical triads, ϵ_{ijk} and ε on the other hand *are* affected by the handedness of e^a_i. Γ^2_a and Γ^3_a can be obtained by permutations of Eq. (4.7).

As is usual in LQC, we will now use the fiducial triads and co-triads in order to introduce a convenient parametrization of the phase space variables E^a_i and A^i_a. Because we have restricted ourselves to the diagonal model and these fields are symmetric under the Bianchi IX group, from each equivalence class of gauge related phase space variables we can choose a pair of the form

$$E^a_i = \frac{p_i}{\ell_o^2}\sqrt{\mathring{q}}\, \mathring{e}^a_i \qquad \text{and} \qquad A^i_a = \frac{c^i}{\ell_o}\mathring{\omega}^i_a, \tag{4.8}$$

where, as spelled out in footnote 3, there is no sum over i. Note that the length ℓ_o plays a similar role to that of the lengths of the fiducial cell in noncompact space-times in terms of the form of the basic variables (A, E). In this case the manifold is compact and there is no fiducial cell.

It is straightforward to relate the scale factors a_i to the p_i:

$$p_1 = \text{sgn}(a_1)|a_2 a_3|\ell_o^2\,, \qquad p_2 = \text{sgn}(a_2)|a_1 a_3|\ell_o^2\,, \qquad p_3 = \text{sgn}(a_3)|a_1 a_2|\ell_o^2\,, \tag{4.9}$$

it follows that $\sqrt{|q|} = \sqrt{|p_1 p_2 p_3|}V_o^{-1}\sqrt{\mathring{q}}$.

Thus, a point in the phase space is now coordinatized by six real numbers (p_i, c^i). One can use the symplectic structure in full general relativity to induce a symplectic structure on the six-dimensional phase space. The nonzero Poisson brackets are given by

$$\{c_i,\, p_j\} \;=\; 8\pi G\gamma\, \delta_{ij}\,, \tag{4.10}$$

where γ is the Barbero-Immirzi parameter.

Our choice in Eq. (4.8) of physical triads and connections has fixed the internal gauge as well as the diffeomorphism freedom. Furthermore, it is easy to explicitly verify that the Gauss and the diffeomorphism constraints are automatically satisfied. Thus we are left with the Hamiltonian constraint

$$\mathcal{C}_H = \int_{\mathcal{M}} \left[\frac{-NE_i^a E_j^b}{16\pi G\gamma^2\sqrt{|q|}} \epsilon^{ij}{}_k \Big(F_{ab}{}^k - (1+\gamma^2)\Omega_{ab}{}^k \Big) + N\mathcal{H}_{\rm matt} \right] \mathrm{d}^3x \approx 0, \quad (4.11)$$

where $F_{ab}{}^k$ and $\Omega_{ab}{}^k$ are the curvatures of A_a^i and Γ_a^i respectively, while $\mathcal{H}_{\rm matt}$ is the matter Hamiltonian density. The ≈ 0 indicates that $\mathcal{C}_H$ is a constraint and must vanish for physical solutions. Since we are most interested in the gravitational sector, our matter field will consist only of a massless scalar field T which will later serve as a relational time variable à la Liebniz. (Additional matter fields can be incorporated in a straightforward manner, modulo possible intricacies of essential self-adjointness.) Thus,

$$\mathcal{H}_{\rm matt} = \frac{1}{2}\frac{p_T^2}{\sqrt{|q|}}. \quad (4.12)$$

Since we want to use the massless scalar field as relational time, it is convenient to use a harmonic-time gauge, i.e., assume that the time coordinate τ satisfies $\Box\tau = 0$. The corresponding lapse function is $N = \sqrt{|p_1p_2p_3|}$. With this choice, the Hamiltonian constraint simplifies considerably.

In terms of p_i, the first component of the spin connection is given by

$$\Gamma_a^1 = \frac{\varepsilon}{r_o}\left(\frac{p_2p_3}{p_1^2} - \frac{p_2}{p_3} - \frac{p_3}{p_2}\right)\mathring{\omega}_a^1, \quad (4.13)$$

the other two spin connection components can be obtained via permutations. The curvature of Γ_a^i is in turn

$$\begin{aligned} \Omega_{ab}{}^1 &= 2\partial_{[a}\Gamma^1_{b]} + \epsilon^1{}_{jk}\Gamma_a^j\Gamma_b^k \\ &= \frac{2\varepsilon}{r_o^2}\left(3\frac{p_2p_3}{p_1^2} + 2\frac{p_1^2}{p_2p_3} - 2\frac{p_2}{p_3} - 2\frac{p_3}{p_2} - \frac{p_1^2p_2}{p_3^3} - \frac{p_1^2p_3}{p_2^3}\right)\mathring{\omega}^2_{[a}\mathring{\omega}^3_{b]}, \end{aligned} \quad (4.14)$$

the other components of $\Omega_{ab}{}^k$ can again be obtained via permutations.

Finally, it is straightforward to calculate the curvature of A_a^i. For example,

$$\begin{aligned} F_{ab}{}^1 &= 2\partial_{[a}A_{b]}^1 + \epsilon^1{}_{jk}A_a^jA_b^k \\ &= 2\left(\frac{2c_1}{\ell_o r_o} + \frac{\varepsilon c_2 c_3}{\ell_o^2}\right)\mathring{\omega}_{[a}^2\mathring{\omega}_{b]}^3. \end{aligned} \tag{4.15}$$

Using these results, one finds that the Hamiltonian constraint of Eq. (4.11) gives

$$\begin{aligned} \mathcal{C}_H = &-\frac{1}{8\pi G\gamma^2}\Bigg(p_1p_2c_1c_2 + p_2p_3c_2c_3 + p_3p_1c_3c_1 + \frac{2\ell_o\varepsilon}{r_o}(p_1p_2c_3 + p_2p_3c_1 + p_3p_1c_2) \\ &+ \frac{\ell_o^2}{r_o^2}(1+\gamma^2)\left[2p_1^2 + 2p_2^2 + 2p_3^2 - \left(\frac{p_1p_2}{p_3}\right)^2 - \left(\frac{p_2p_3}{p_1}\right)^2 - \left(\frac{p_3p_1}{p_2}\right)^2\right]\Bigg) \\ &+ \frac{1}{2}p_T^2 \approx 0. \end{aligned} \tag{4.16}$$

Note that the constraint for the closed isotropic case is recovered for $p_1 = p_2 = p_3$ while the Bianchi I constraint is recovered in the limit $r_o \to \infty$ or, equivalently, $\ell_o \to 0$. We will take advantage of this correspondence and set $r_o = 2$ for the remainder of the chapter. The Bianchi I limit can be obtained by taking $\ell_o \to 0$.

One can now derive the time evolution of any classical observable $\mathcal{O}$ by taking its Poisson bracket with $\mathcal{C}_H$:

$$\dot{\mathcal{O}} = \{\mathcal{O}, \mathcal{C}_H\}, \tag{4.17}$$

where the 'dot' stands for derivative with respect to the harmonic time τ. This gives

$$\dot{p_1} = \frac{p_1}{\gamma}\left(p_2c_2 + p_3c_3 + \ell_o\varepsilon\frac{p_2p_3}{p_1}\right), \tag{4.18}$$

$$\begin{aligned} \dot{c_1} = &-\frac{1}{\gamma}\Bigg(p_2c_1c_2 + p_3c_1c_3 + \ell_o\varepsilon(p_2c_3 + p_3c_2) \\ &+ \ell_o^2(1+\gamma^2)\left(p_1 + \frac{p_2^2p_3^2}{2p_1^3} - \frac{p_1p_2^2}{2p_3^2} - \frac{p_1p_3^2}{2p_3^2}\right)\Bigg). \end{aligned} \tag{4.19}$$

As usual, the other equations of motion can be obtained by permutations. Any initial data satisfying the Hamiltonian constraint can be evolved by these equations of motion. It is particularly interesting to study the Hubble rates H_i which are given by

$$H_i = \frac{1}{a_i}\frac{\mathrm{d}a_i}{\mathrm{d}t}, \tag{4.20}$$

where t is the proper time and is related to the harmonic time τ (which is the time coordinate used until now) by

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{1}{\sqrt{|p_1p_2p_3|}}\frac{\mathrm{d}}{\mathrm{d}\tau}. \tag{4.21}$$

It follows that the Hubble rates are related to the (c_i, p_i) by, e.g.,

$$c_1p_1 = \gamma\sqrt{|p_1p_2p_3|}H_1 + \frac{\ell_o}{2}\left(\frac{p_2p_3}{p_1} - \frac{p_1p_2}{p_3} - \frac{p_1p_3}{p_2}\right). \tag{4.22}$$

The mean Hubble rate H of the mean scale factor $a = (a_1a_2a_3)^{1/3}$ is given by

$$H = \frac{1}{a}\frac{\mathrm{d}a}{\mathrm{d}t} = \frac{1}{3}(H_1 + H_2 + H_3), \tag{4.23}$$

and the Friedmann equation is

$$H^2 = \frac{8\pi G}{3}\rho + \frac{1}{6}\sigma^2 - \frac{\ell_o^2}{12}V(p), \tag{4.24}$$

where the energy density of the scalar field is $\rho = p_T^2/2|p_1p_2p_3|$, the shear term is given by

$$\sigma^2 = \frac{1}{3}[(H_1 - H_2)^2 + (H_2 - H_3)^2 + (H_3 - H_1)^2], \tag{4.25}$$

and the potential is

$$V(p) = \frac{1}{p_1p_2p_3}\left[2(p_1^2 + p_2^2 + p_3^2) - \left(\frac{p_2p_3}{p_1}\right)^2 - \left(\frac{p_3p_1}{p_2}\right)^2 - \left(\frac{p_1p_2}{p_3}\right)^2\right]. \tag{4.26}$$

Clearly, these dynamics are quite complex already at the classical level and, as mentioned in the introduction, become chaotic as a singularity is approached. The one exception is the case when the matter field is a massless scalar field which is precisely what is considered here. In this case, as the singularity is approached, the Friedmann equation will become asymptotically velocity term dominated (AVTD) if the scalar field's momentum is large enough. In this case, the potential can safely be neglected [92]. Thus, as the singularity is approached, the dynamics are the same as those of the Bianchi I space-time with a massless scalar field. This behaviour will be important for the study of the effective equations later. However, the quantum Hamiltonian constraint operator derived in the following section will hold regardless of the scalar field's momentum and it will be relatively straightforward to extend it for other types of matter fields as well.

Finally, before moving on to the quantum theory, let us consider the parity transformation Π_k which flips the kth *physical* triad vector e^a_k. (Keep in mind that this transformation does not act on any of the fiducial quantities which carry the label o.) These correspond to residual discrete gauge transformations related to the orientation of the physical triads. Under this map, we have: $q_{ab} \to q_{ab}$, $\epsilon_{abc} \to \epsilon_{abc}$ but $\epsilon_{ijk} \to -\epsilon_{ijk}$, $\varepsilon \to -\varepsilon$. The canonical variables c_i, p_i transform as proper internal vectors and co-vectors. For example,

$$\Pi_1(c_1, c_2, c_3) \to (-c_1, c_2, c_3) \qquad \text{and} \qquad \Pi_1(p_1, p_2, p_3) \to (-p_1, p_2, p_3)\,. \tag{4.27}$$

Consequently, both the symplectic structure and the Hamiltonian constraint are left invariant under any of the parity maps Π_k.

The Hamiltonian description given in this section will serve as the starting point for the loop quantization performed in the next section.

4.3 Quantum Theory

This section is divided into two parts. In the first, we discuss the kinematics of the model while in the second we introduce the Hamiltonian constraint operator using the groundwork laid out in Chapters 2 and 3 and describe its action on physical states.

4.3.1 LQC Kinematics

The kinematics for the LQC of Bianchi IX models are identical to those of the Bianchi II models, but we will briefly present the kinematics here as well for the sake of completeness.

The elementary functions on the classical phase space that have unambiguous analogs in the quantum theory are the momenta p_i and holonomies $h_k^{(\mu)}$ of the gravitational connection A_a^i along the integral curves of $\mathring{e}_k^a$ of length $\mu\ell_o$ with respect to the fiducial metric $\mathring{q}_{ab}$. These holonomies are given by

$$h_k^{(\mu)}(c_1, c_2, c_3) = \exp\left(\mu c_k \tau_k\right) = \cos\frac{\mu c_k}{2}\mathbb{I} + 2\sin\frac{\mu c_k}{2}\tau_k, \tag{4.28}$$

where the τ_k are $-i/2$ times the Pauli matrices. This family of holonomies is completely determined by the almost periodic functions $\exp(i\mu c_k)$ of the connection. These almost periodic functions will be the elementary configuration variables which will be promoted unambiguously to operators in the quantum theory.

It is simplest to use the p-representation to specify the gravitational sector $\mathcal{H}_{\text{kin}}^{\text{grav}}$ of the kinematic Hilbert space. The basis is orthonormal in the sense that

$$\langle p_1, p_2, p_3 | p_1', p_2', p_3' \rangle = \delta_{p_1 p_1'} \delta_{p_2 p_2'} \delta_{p_3 p_3'}\,, \tag{4.29}$$

where the right side features Kronecker delta symbols rather than Dirac delta distributions. Kinematical states consist of countable linear combinations

$$|\Psi\rangle \;=\; \sum_{p_1, p_2, p_3} \Psi(p_1, p_2, p_3) |p_1, p_2, p_3\rangle \tag{4.30}$$

of these basis states with finite norm

$$||\Psi||^2 \;=\; \sum_{p_1, p_2, p_3} |\Psi(p_1, p_2, p_3)|^2. \tag{4.31}$$

Next, recall that on the classical phase space the three reflections $\Pi_i:\; e_i^a \to -e_i^a$ are large gauge transformations under which physics does not change since both the metric and the extrinsic curvature are left invariant. These large gauge transformations have a natural induced action, denoted by $\hat{\Pi}_i$, on the space of wave functions $\Psi(p_1, p_2, p_3)$. For example,

$$\hat{\Pi}_1 \Psi(p_1, p_2, p_3) = \Psi(-p_1, p_2, p_3). \tag{4.32}$$

Since $\hat{\Pi}_i^2$ is the identity, for each i the group of these large gauge transformations is simply $\mathbb{Z}_2$. As in Yang-Mills theory, physical states belong to its irreducible representation. For definiteness, as in the isotropic and the Bianchi type I and type II models, we will work with the symmetric representation. It then follows that $\mathcal{H}_{\rm kin}^{\rm grav}$ is spanned by wave functions $\Psi(p_1, p_2, p_3)$ which satisfy

$$\Psi(p_1, p_2, p_3) = \Psi(|p_1|, |p_2|, |p_3|) \tag{4.33}$$

and have a finite norm.

The action of the elementary operators on $\mathcal{H}_{\rm kin}^{\rm grav}$ is as follows: the momenta act by multiplication whereas the almost periodic functions in c_i shift the ith argument. For example,

$$[\hat{p}_1 \Psi](p_1, p_2, p_3) = p_1 \, \Psi(p_1, p_2, p_3), \quad \text{and} \tag{4.34}$$

$$\left[\widehat{\exp(i\mu c_1)}\Psi\right](p_1, p_2, p_3) = \Psi(p_1 - 8\pi\gamma G\hbar\mu, p_2, p_3)\,. \tag{4.35}$$

The expressions for $\hat{p}_2, \widehat{\exp(i\mu c_2)}, \hat{p}_3$ and $\widehat{\exp(i\mu c_3)}$ are analogous. Finally, we must define the operator $\hat{\varepsilon}$ since ε features in the expression of the Hamiltonian constraint. As in Chapter 3, we define

$$\hat{\varepsilon}\,|p_1, p_2, p_3\rangle := \begin{cases} \;\;|p_1, p_2, p_3\rangle \text{ if } p_1p_2p_3 \geq 0, \\ -\,|p_1, p_2, p_3\rangle \text{ if } p_1p_2p_3 < 0. \end{cases} \tag{4.36}$$

Finally, the full kinematical Hilbert space $\mathcal{H}_{\rm kin}$ will be the tensor product $\mathcal{H}_{\rm kin} = \mathcal{H}_{\rm kin}^{\rm grav} \otimes \mathcal{H}_{\rm kin}^{\rm matt}$, where $\mathcal{H}_{\rm kin}^{\rm matt} = L^2(\mathbb{R}, dT)$ is the matter kinematical Hilbert space for the homogeneous scalar field. On $\mathcal{H}_{\rm kin}^{\rm matt}$, $\hat{T}$ will act by multiplication and $\hat{p}_T := -i\hbar {\rm d}_T$ will act by differentiation.

4.3.2 The Quantum Hamiltonian Constraint

To define the quantum Hamiltonian constraint, we must express the classical Hamiltonian constraint in terms of almost periodic functions of the connection which can be directly promoted to operators. This can be done by expressing the field strength ${F_{ab}}^k$ in terms of holonomies for isotropic and/or spatially flat space-times, see, e.g., [34, 46, 47, 86]. However, this is not possible for space-times which are both anisotropic and spatially curved such as the Bianchi type II and type IX models. In this case we need to extend the strategy: the connection itself —rather than the field strength— has to be expressed in terms of holonomies. This task was carried out in Chapter 3. The connection operator is given by

$$\hat{c}_k = \frac{\widehat{\sin(\bar{\mu}_k c_k)}}{\bar{\mu}_k}, \tag{4.37}$$

where

$$\bar{\mu}_1 = \sqrt{\frac{|p_1|\Delta\,\ell_{\rm Pl}^2}{|p_2 p_3|}}, \qquad \bar{\mu}_2 = \sqrt{\frac{|p_2|\Delta\,\ell_{\rm Pl}^2}{|p_1 p_3|}}, \qquad \bar{\mu}_3 = \sqrt{\frac{|p_3|\Delta\,\ell_{\rm Pl}^2}{|p_1 p_2|}}, \tag{4.38}$$

and $\Delta\,\ell_{\rm Pl}^2 = 4\sqrt{3}\pi\gamma\,\ell_{\rm Pl}^2$ is the 'area gap'. Note that the choice for this operator is motivated by LQG: it is obtained by expressing the connection in terms of holonomies, a procedure commonly used in LQG, and then ensuring that this approach is equivalent to what is done for simpler cosmological models where it is the field strength which is expressed in terms of holonomies. Although the precise value of the area gap may change as the relation between LQG and LQC is better understood, the form of $\bar{\mu}_i$ in terms of the p_i is necessary in order to obtain the correct infrared, low curvature behaviour.

Using the connection operator, it is possible to promote the classical Hamiltonian constraint in Eq. (4.16) to an operator. Ignoring factor ordering ambiguities and inverse triad operators for the moment, $\hat{\mathcal{C}}_H$ is given by

$$\begin{aligned}
\hat{\mathcal{C}}_H = &-\frac{1}{8\pi G\gamma^2\Delta\ell_{\rm Pl}^2}\Bigg[p_1p_2|p_3|\sin\bar{\mu}_1c_1\sin\bar{\mu}_2c_2 + |p_1|p_2p_3\sin\bar{\mu}_2c_2\sin\bar{\mu}_3c_3 \\
&+ p_1|p_2|p_3\sin\bar{\mu}_3c_3\sin\bar{\mu}_1c_1\Bigg] - \frac{\ell_o\hat{\varepsilon}}{8\pi G\gamma^2\sqrt{\Delta}\ell_{\rm Pl}}\Bigg[p_1p_2\sqrt{\frac{|p_1p_2|}{|p_3|}}\sin\bar{\mu}_3c_3 \\
&+ p_2p_3\sqrt{\frac{|p_2p_3|}{|p_1|}}\sin\bar{\mu}_1c_1 + p_3p_1\sqrt{\frac{|p_3p_1|}{|p_2|}}\sin\bar{\mu}_2c_2\Bigg] \\
&- \frac{\ell_o^2(1+\gamma^2)}{32\pi G\gamma^2}\Bigg[2\left(p_1^2+p_2^2+p_3^2\right) - \left(\frac{p_1p_2}{p_3}\right)^2 - \left(\frac{p_2p_3}{p_1}\right)^2 - \left(\frac{p_3p_1}{p_2}\right)^2\Bigg] \\
&+ \frac{1}{2}\hat{p}_T^2,
\end{aligned} \tag{4.39}$$

where for simplicity of notation here and in what follows we have dropped the hats on the p_i and $\sin \bar{\mu}_i c_i$ operators.

To obtain the action of the $\sin \bar{\mu}_i c_i$ operators [or, equivalently, the $\exp(i\bar{\mu}_i c_i)$ operators] we will use the same strategy as in Chapter 2. As shown there, it is simplest to introduce the dimensionless variables

$$\lambda_i = \frac{\mathrm{sgn}(p_i)\sqrt{|p_i|}}{(4\pi\gamma\sqrt{\Delta}\ell_{\mathrm{Pl}}^3)^{1/3}}\,. \tag{4.40}$$

Then the kets $|\lambda_1, \lambda_2, \lambda_3\rangle$ constitute an orthonormal basis in which the operators p_k are diagonal

$$p_k|\lambda_1, \lambda_2, \lambda_3\rangle \;=\; [\mathrm{sgn}(\lambda_k)(4\pi\gamma\sqrt{\Delta}\ell_{\mathrm{Pl}}^3)^{2/3}\lambda_k^2]\;|\lambda_1, \lambda_2, \lambda_3\rangle\,, \tag{4.41}$$

and quantum states are represented by functions $\Psi(\lambda_1, \lambda_2, \lambda_3)$. Then the operator $e^{i\bar{\mu}_1 c_1}$ acts by shifting the wave function,

$$\begin{aligned}\left[e^{i\bar{\mu}_1 c_1}\,\Psi\right](\lambda_1, \lambda_2, \lambda_3) &= \Psi(\lambda_1 - \frac{1}{|\lambda_2\lambda_3|}, \lambda_2, \lambda_3)\\ &= \Psi(\frac{v - 2\mathrm{sgn}(\lambda_2\lambda_3)}{v}\cdot\,\lambda_1, \lambda_2, \lambda_3),\end{aligned} \tag{4.42}$$

where we have introduced the variable $v = 2\lambda_1\lambda_2\lambda_3$ which is proportional to the volume V of the space-time:

$$\hat{V}\,\Psi(\lambda_1, \lambda_2, \lambda_3) \;=\; [2\pi\gamma\sqrt{\Delta}\,|v|\,\ell_{\mathrm{Pl}}^3]\,\Psi(\lambda_1, \lambda_2, \lambda_3). \tag{4.43}$$

The action of the operators $e^{i\bar{\mu}_2 c_2}$ and $e^{i\bar{\mu}_3 c_3}$ is analogous.

We are now ready to write the Hamiltonian constraint explicitly in the λ_i-representation:

$$\hat{\mathcal{C}}_H = \hat{\mathcal{C}}_1 + \hat{\mathcal{C}}_2 + \hat{\mathcal{C}}_3 + \hat{\mathcal{C}}_4 + \tfrac{1}{2}\hat{p}_T^2, \tag{4.44}$$

where, again ignoring factor-ordering issues for the time being,

$$\begin{aligned}\hat{\mathcal{C}}_1 = -\tfrac{1}{2}\pi\hbar\ell_{\mathrm{Pl}}^2 v^2\Big[&\mathrm{sgn}(\lambda_1\lambda_2)\sin\bar{\mu}_1 c_1 \sin\bar{\mu}_2 c_2 + \mathrm{sgn}(\lambda_2\lambda_3)\sin\bar{\mu}_2 c_2 \sin\bar{\mu}_3 c_3\\ &+ \mathrm{sgn}(\lambda_3\lambda_1)\sin\bar{\mu}_3 c_3 \sin\bar{\mu}_1 c_1\Big];\end{aligned} \tag{4.45}$$

$$\hat{\mathcal{C}}_2 = -2\pi\sqrt{\Delta}\hbar\ell_{\rm Pl}^3\ell_o\hat{\varepsilon}\Big[(\lambda_1\lambda_2)^3\frac{1}{\sqrt{|p_3|}}\sin\bar{\mu}_3c_3 + (\lambda_2\lambda_3)^3\frac{1}{\sqrt{|p_1|}}\sin\bar{\mu}_1c_1 + (\lambda_3\lambda_1)^3\frac{1}{\sqrt{|p_2|}}\sin\bar{\mu}_2c_2\Big]; \tag{4.46}$$

$$\hat{\mathcal{C}}_3 = -\frac{(4\pi\gamma\sqrt{\Delta})^{1/3}\sqrt{\Delta}\hbar\ell_{\rm Pl}^2}{4\gamma}\ell_o^2(1+\gamma^2)\Big[\lambda_1^4+\lambda_2^4+\lambda_3^4\Big]; \tag{4.47}$$

$$\hat{\mathcal{C}}_4 = \tfrac{1}{2}(16\pi^2\gamma^2\Delta)^{1/3}\pi\Delta\hbar\ell_{\rm Pl}^6\ell_o^2(1+\gamma^2)\left[(\lambda_1\lambda_2)^4\cdot\left(\frac{1}{p_3}\right)^2 + (\lambda_2\lambda_3)^4\cdot\left(\frac{1}{p_1}\right)^2 + (\lambda_3\lambda_1)^4\cdot\left(\frac{1}{p_2}\right)^2\right]. \tag{4.48}$$

It will be straightforward to deal with $\hat{\mathcal{C}}_H$ since the terms in $\hat{\mathcal{C}}_1$ are the exact terms that appear in the Bianchi I model and have already been studied in Chapter 2 while the terms in $\hat{\mathcal{C}}_2$ and $\hat{\mathcal{C}}_4$ are of the same form as some of the terms in the Bianchi II model considered in Chapter 3. Finally, the only new terms —those in $\hat{\mathcal{C}}_3$— act by multiplication and will not cause any difficulty.

All of the terms will be factor-ordered in a symmetric manner. For example, in agreement with the choices made in the previous 2 chapters (and dropping the numerical prefactors), the first term in $\hat{\mathcal{C}}_1$ will be factor-ordered as

$$\sqrt{|v|}\Bigg[(\sin\bar{\mu}_1c_1{\rm sgn}\lambda_1 + {\rm sgn}\lambda_1\sin\bar{\mu}_1c_1)|v|(\sin\bar{\mu}_2c_2{\rm sgn}\lambda_2 + {\rm sgn}\lambda_2\sin\bar{\mu}_2c_2) + (\sin\bar{\mu}_2c_2{\rm sgn}\lambda_2 + {\rm sgn}\lambda_2\sin\bar{\mu}_2c_2)|v|(\sin\bar{\mu}_1c_1{\rm sgn}\lambda_1 + {\rm sgn}\lambda_1\sin\bar{\mu}_1c_1)\Bigg]\sqrt{|v|}, \tag{4.49}$$

while the first term in $\hat{\mathcal{C}}_2$ will be

$$(\lambda_1\lambda_2)^3\frac{1}{|p_3|^{1/4}}\Big[\hat{\varepsilon}\sin\bar{\mu}_3c_3 + \sin\bar{\mu}_3c_3\hat{\varepsilon}\Big]\frac{1}{|p_3|^{1/4}}. \tag{4.50}$$

Since all of the components in each term in $\hat{\mathcal{C}}_3$ and $\hat{\mathcal{C}}_4$ commute, there are no factor-ordering choices to be made for these terms.

Recall, that the inverse volume operators can be obtained by using a variation on the Thiemann inverse triad identities [119, 120] (see Chapter 3 for details):

$$\widehat{|p_1|^{-1/4}}\,|\lambda_1,\lambda_2,\lambda_3\rangle = \frac{\sqrt{2}\mathrm{sgn}(\lambda_1)\,\sqrt{|\lambda_2\lambda_3|}}{(4\pi\gamma\sqrt{\Delta}\ell_{\mathrm{Pl}}^3)^{1/6}}\Big(\sqrt{|v+\mathrm{sgn}(\lambda_2\lambda_3)|} - \sqrt{|v-\mathrm{sgn}(\lambda_2\lambda_3)|}\Big)\,|\lambda_1,\lambda_2,\lambda_3\rangle. \tag{4.51}$$

This operator is diagonal in the eigenbasis $|\lambda_1,\lambda_2,\lambda_3\rangle$ and, on eigenkets with large volume, the eigenvalue is indeed well approximated by $|p_1|^{-1/4}$, whence on semi-classical states it behaves as the inverse of $|\hat{p}|^{1/4}$, just as one would hope. Nonetheless, there are interesting nontrivialities in the Planck regime, the most important one being that the inverse triad operator annihilates any ket $|\lambda_1,\lambda_2,\lambda_3\rangle$ where $v = 2\lambda_1\lambda_2\lambda_3 = 0$.

Finally, the other inverse triad operator which is necessary for the study of Bianchi IX models can be defined by

$$\widehat{p_i^{-2}} := \left(\widehat{|p_i|^{-1/4}}\right)^8. \tag{4.52}$$

As in the Bianchi I model, the action simplifies if we replace $(\lambda_i,\lambda_j,\lambda_k)$ by (λ_i,λ_j,v)[4]. Because of the high symmetry of the Bianchi IX model, it does not matter which of the λ_i is replaced; we will choose to replace λ_3 by v here. This change of variables would be nontrivial if, as in the Wheeler-DeWitt theory, we had used the Lesbegue measure in the gravitational sector. However, it is quite tame here because the norms are defined using a discrete measure. The inner product on $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$ is now given by

$$\langle\Psi_1|\Psi_2\rangle_{\mathrm{kin}} = \sum_{\lambda_1,\lambda_2,v} \bar{\Psi}_1(\lambda_1,\lambda_2,v)\,\Psi_2(\lambda_1,\lambda_2,v), \tag{4.53}$$

and states are symmetric under the action of $\hat{\Pi}_k$. In Appendix A, it is shown that under the action of the $\hat{\Pi}_i$, the operators $\sin\bar{\mu}_i c_i$ have the same transformation properties as c_i under the reflections Π_i in the classical theory. As a consequence, $\hat{\mathcal{C}}_H$ is also reflection symmetric[5]. Therefore, its action is well-defined on $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$: $\hat{\mathcal{C}}_H$

[4] This cannot be done for states where $\lambda_1\lambda_2\lambda_3 = 0$ but since these states decouple under the action of $\hat{\mathcal{C}}_H$, we can restrict our attention solely to states where $\lambda_1\lambda_2\lambda_3 \neq 0$.

[5] Note that although $\hat{\Pi}_i\hat{\varepsilon}\hat{\Pi}_i = -\hat{\varepsilon}$ (recall that classically $\varepsilon \to -\varepsilon$ under a parity transformation)

is a densely defined, symmetric operator on this Hilbert space. In the flat FLRW and Bianchi I cases, its analog has been shown to be essentially self-adjoint [40, 41]. In what follows we will assume that $\hat{\mathcal{C}}_H$ is essentially self-adjoint on $\mathcal{H}_{\rm kin}^{\rm grav}$ and work with its self-adjoint extension.

We can now study the action of $\hat{\mathcal{C}}_H$ on a wave function. For a complete derivation of the action of each term in the constraint, see Chapters 2 and 3.

It is straightforward to write down the full Hamiltonian constraint on $\mathcal{H}_{\rm kin}^{\rm grav}$:

$$-\hbar^2\,\partial_T^2\,\Psi(\lambda_2,\lambda_3,v;T)=\hat{\Theta}\,\Psi(\lambda_2,\lambda_3,v;T),\quad \text{where}\quad \hat{\Theta}=-2\hat{\mathcal{C}}_{\rm grav}. \tag{4.54}$$

As in the isotropic case [33], one can obtain the physical Hilbert space $\mathcal{H}_{\rm phy}$ by a group averaging procedure and the final result is completely analogous. Elements of $\mathcal{H}_{\rm phy}$ consist of 'positive frequency' solutions to (4.54), i.e., solutions to

$$-i\hbar\partial_T\Psi(\lambda_1,\lambda_2,v;T)\;=\;\sqrt{|\hat{\Theta}|}\,\Psi(\lambda_1,\lambda_2,v;T)\,, \tag{4.55}$$

which are symmetric under the three reflection maps $\hat{\Pi}_i$:

$$\Psi(\lambda_1,\lambda_2,v;\,T)=\Psi(|\lambda_1|,|\lambda_2|,|v|;\,T)\,. \tag{4.56}$$

The scalar product is simply given by

$$\begin{aligned}\langle\Psi_1|\Psi_2\rangle_{\rm phys} &= \langle\Psi_1(\lambda_1,\lambda_2,v;T_o)|\Psi_2(\lambda_1,\lambda_2,v;T_o)\rangle_{\rm kin}\\ &= \sum_{\lambda_1,\lambda_2,v}\bar{\Psi}_1(\lambda_1,\lambda_2,v;T_o)\,\Psi_2(\lambda_1,\lambda_2,v;T_o),\end{aligned} \tag{4.57}$$

where T_o is any "instant" of internal time T.

Since elements of $\mathcal{H}_{\rm kin}^{\rm grav}$ are invariant under the three parity maps $\hat{\Pi}_k$ and the Hamiltonian constraint satisfies $\hat{\Pi}_k\,\hat{\mathcal{C}}_{\rm grav}\hat{\Pi}_k=\hat{\mathcal{C}}_{\rm grav}$, knowledge of the restriction of the image $\hat{\mathcal{C}}_{\rm grav}\Psi$ of Ψ to the positive octant suffices to determine $\hat{\mathcal{C}}_{\rm grav}\Psi$ completely. Therefore, in the remainder of this section we will restrict the argument of $\hat{\mathcal{C}}_H\Psi$

only when $v\neq 0$, in the $v=0$ case the wave function is annihilated by the gravitational part of the Hamiltonian constraint $\hat{\mathcal{C}}_{\rm grav}$ and therefore $\hat{\Pi}_i\hat{\mathcal{C}}_{\rm grav}\hat{\Pi}_i|\Psi_{\rm sing}\rangle=0=\hat{\mathcal{C}}_{\rm grav}|\Psi_{\rm sing}\rangle$ where $|\Psi_{\rm sing}\rangle$ is a state that only has support on $v=0$. It is then straightforward to show that $\hat{\Pi}_i\hat{\mathcal{C}}_H\hat{\Pi}_i|\Psi\rangle=\hat{\mathcal{C}}_H|\Psi\rangle$ for all wave functions.

to the positive octant. The full action is simply given by

$$\big(\hat{\mathcal{C}}_{\rm grav}\Psi\big)(\lambda_1,\lambda_2,v)=\big(\hat{\mathcal{C}}_{\rm grav}\Psi\big)(|\lambda_1|,|\lambda_2|,|v|). \tag{4.58}$$

Since all states with $v=0$ are annihilated by $\hat{\mathcal{C}}_{\rm grav}$, their evolution is trivial:

$$\partial_T^2\,\Psi(\lambda_1,\lambda_2,v=0;T)=0\,. \tag{4.59}$$

Such states correspond to classical geometries which are singular and therefore we will call these states 'singular' even though they are well-defined in the quantum theory. Nonsingular states on the other hand are physically much more interesting. On them, the explicit form of the full constraint is given by:

$$\begin{aligned}\partial_T^2\,\Psi=\pi G\Bigg\{&\frac{\sqrt{v}}{8}\Big[(v+2)\sqrt{v+4}\,\Psi_4^+-(v+2)\sqrt{v}\,\Psi_0^+\\&-\theta_{v-2}(v-2)\sqrt{v}\,\Psi_0^-+\theta_{v-4}(v-2)\sqrt{|v-4|}\,\Psi_4^-\Big]\\&-\frac{2i\ell_o\sqrt{\Delta}}{(4\pi\gamma\sqrt{\Delta})^{1/3}}\Big[\sqrt{v+1}-\sqrt{|v-1|}\Big]\Big(\Phi^+-\theta_{v-2}\Phi^-\Big)\\&+\frac{8\Delta\ell_o^2(1+\gamma^2)}{(4\pi\gamma\sqrt{\Delta})^{2/3}}\Big[(\sqrt{v+1}-\sqrt{|v-1|})^8\Big((\lambda_1\lambda_2)^8+(\lambda_2\lambda_3)^8\\&\quad+(\lambda_3\lambda_1)^8\Big)-\frac{1}{8}\big(\lambda_1^4+\lambda_2^4+\lambda_3^4\big)\Big]\,\Psi\Bigg\},\end{aligned} \tag{4.60}$$

where we have dropped the arguments which are all $(\lambda_1,\lambda_2,v;T)$. Note that, as usual, the step function kills any terms that would allow the positive octant to interact with any of the other octants, this is a direct consequence of the factor-ordering choices made earlier.

The $\Psi_{0,4}^{\pm}$ are defined as follows:

$$\begin{aligned}\Psi_n^{\pm}(\lambda_1,\lambda_2,v;T)=\;&\Psi\left(\tfrac{v\pm n}{v\pm 2}\cdot\lambda_1,\tfrac{v\pm 2}{v}\cdot\lambda_2,v\pm n;T\right)+\Psi\left(\tfrac{v\pm n}{v\pm 2}\cdot\lambda_1,\lambda_2,v\pm n;T\right)\\&+\Psi\left(\tfrac{v\pm 2}{v}\cdot\lambda_1,\tfrac{v\pm n}{v\pm 2}\cdot\lambda_2,v\pm n;T\right)+\Psi\left(\tfrac{v\pm 2}{v}\cdot\lambda_1,\lambda_2,v\pm n;T\right)\\&+\Psi\left(\lambda_1,\tfrac{v\pm 2}{v}\cdot\lambda_2,v\pm n;T\right)+\Psi\left(\lambda_1,\tfrac{v\pm n}{v\pm 2}\cdot\lambda_2,v\pm n;T\right),\end{aligned} \tag{4.61}$$

while the $\Phi^{\pm}$ are given by

$$\Phi^{\pm}(\lambda_1, \lambda_2, v; T) = \left(\sqrt{|v \pm 2 + 1|} - \sqrt{|v \pm 2 - 1|}\right) \cdot \Bigg[\lambda_2^4 \lambda_3^4 \, \Psi\Big(\tfrac{v \pm 2}{v} \cdot \lambda_1, \lambda_2, v \pm 2; T\Big) + \lambda_3^4 \lambda_1^4 \, \Psi\Big(\lambda_1, \tfrac{v \pm 2}{v} \cdot \lambda_2, v \pm 2; T\Big) + \lambda_1^4 \lambda_2^4 \, \Psi\Big(\lambda_1, \lambda_2, v \pm 2; T\Big)\Bigg]. \quad (4.62)$$

As expected, the quantum dynamics of the Bianchi IX model reduces to that of the Bianchi I model discussed in Chapter 2 in the limit $\ell_o \rightarrow 0$ in Eq. (4.60).

Equation (4.60) also immediately implies that the steps in v are uniform: the argument of the wave function only involves $v-4, v-2, v, v+2$ and $v+4$. Thus, there is a superselection in v. For each $\epsilon \in [0, 2)$, we can introduce a lattice $\mathcal{L}_\epsilon$ of points $v = 2n + \epsilon$. Then the quantum evolution —and the action of the Dirac observables $\hat{p}_T$ and $\hat{V}|_T$ commonly used in LQC— preserves the subspaces $\mathcal{H}^\epsilon_{\rm phy}$ consisting of states with support in v on $\mathcal{L}_\epsilon$. The most interesting lattice is the one corresponding to $\epsilon = 0$ since it includes the classically singular points $v = 0$.

The form of the action of the Hamiltonian constraint operator also shows that the classical singularity is resolved. Using the scalar field T as time, we find that if one starts with a wave function which only has support on singular states, that wave function does not evolve in T and therefore will always only have support on singular states.

On the other hand, a state which does not have any support on the singular subspace will never have support on it. Restricting our argument to the positive octant for the sake of simplicity (it can easily be generalized to the other octants), it is easy to see that to go from $\lambda_1, \lambda_2, v > 0$ to $v = 0$, one must either have $v = 2$ and then Φ^- will give a term with $v = 0$ or have $v = 4$ and then Ψ_4^- will give a term with $v = 0$. However, the prefactors in front of Φ^- vanish for $v = 2$ just as the prefactors in front of Ψ_4^- vanish for $v = 4$. Because of this, it is impossible for a wave function with no support on singular states to ever gain support on a singular state.

This shows that singular states decouple from nonsingular states under the relational T dynamics given by Eqs. (4.59) and (4.60). In other words, if one starts with a nonsingular state at some 'time' T_o, it will remain nonsingular throughout its evolution. It is in this (rather strong) sense that the singularity is resolved.

4.4 Effective Equations

In isotropic models, effective equations obtained via an embedding approach [37, 38] provide an excellent approximation to the full quantum evolution of states which are Gaussians at late times, even in the $\Lambda \neq 0$ as well as k=±1 cases where the models are not exactly soluble. In this section we will derive such effective equations for the Bianchi IX model (although we will ignore the effect of fluctutations in this work) in order to gain qualitative insights into modifications of the equations of motion due to quantum geometry effects.

To obtain the effective equations we can restrict our attention to the positive octant of the classical phase space (where $\varepsilon = 1$) without loss of generality. Then the quantum corrected Hamiltonian constraint is given by the classical analogue of Eq. (4.39):

$$\frac{p_T^2}{2} + \mathcal{C}_{\rm grav}^{\rm eff} = 0, \tag{4.63}$$

where[6]

$$\begin{aligned}
\mathcal{C}_{\rm grav}^{\rm eff} = &- \frac{p_1 p_2 p_3}{8\pi G \gamma^2 \Delta \ell_{\rm Pl}^2} \Big[\sin \bar{\mu}_1 c_1 \sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_2 c_2 \sin \bar{\mu}_3 c_3 + \sin \bar{\mu}_3 c_3 \sin \bar{\mu}_1 c_1 \Big] \\
&- \frac{\ell_o}{8\pi G \gamma^2 \sqrt{\Delta} \ell_{\rm Pl}} \left[\frac{(p_1 p_2)^{\frac{3}{2}}}{\sqrt{p_3}} \sin \bar{\mu}_3 c_3 + \frac{(p_2 p_3)^{\frac{3}{2}}}{\sqrt{p_1}} \sin \bar{\mu}_1 c_1 + \frac{(p_3 p_1)^{\frac{3}{2}}}{\sqrt{p_2}} \sin \bar{\mu}_2 c_2 \right] \\
&- \frac{\ell_o^2 (1+\gamma^2)}{32\pi G \gamma^2} \left[2(p_1^2 + p_2^2 + p_3^2) - \left(\frac{p_1 p_2}{p_3}\right)^2 - \left(\frac{p_2 p_3}{p_1}\right)^2 - \left(\frac{p_3 p_1}{p_2}\right)^2 \right].
\end{aligned} \tag{4.64}$$

Using the expressions (4.38) of $\bar{\mu}_k$, it is easy to verify that far away from the classical singularity —more precisely in the regime in which the Hubbles rates H_i are well below the Planck scale— the effective Hamiltonian constraint in Eq. (4.63) is well-approximated by the classical one given in Eq. (4.16).

The effective dynamics are obtained by taking Poisson brackets with the effective Hamiltonian constraint. This gives

$$\dot{p_1} = \gamma^{-1} \left(\frac{p_1^2}{\bar{\mu}_1} (\sin \bar{\mu}_2 c_2 + \sin \bar{\mu}_3 c_3) + \ell_o p_2 p_3 \right) \cos \bar{\mu}_1 c_1; \tag{4.65}$$

[6]Recall that every ℓ_o which appears in the constraint is divided by r_o which has been set to 2. As ℓ_o / r_o is dimensionless, one must ignore ℓ_o when counting units.

$$\begin{aligned}\dot{c_1} = -\frac{1}{\gamma}\Bigg[\frac{p_2 p_3}{\Delta\ell_{\rm Pl}^2}\Bigg(&\sin\bar\mu_1 c_1\sin\bar\mu_2 c_2 + \sin\bar\mu_1 c_1 \sin\bar\mu_3 c_3 + \sin\bar\mu_2 c_2\sin\bar\mu_3 c_3\\ &+\frac{\bar\mu_1 c_1}{2}\cos\bar\mu_1 c_1(\sin\bar\mu_2 c_2+\sin\bar\mu_3 c_3) - \frac{\bar\mu_2 c_2}{2}\cos\bar\mu_2 c_2(\sin\bar\mu_1 c_1 + \sin\bar\mu_3 c_3)\\ &-\frac{\bar\mu_3 c_3}{2}\cos\bar\mu_3 c_3(\sin\bar\mu_1 c_1+\sin\bar\mu_2 c_2)\Bigg) + \ell_o\Bigg(\frac{3}{2\bar\mu_1}\Bigg[\frac{p_1 p_2}{p_3}\sin\bar\mu_3 c_3\\ &+\frac{p_1 p_3}{p_2}\sin\bar\mu_2 c_2 - \frac{p_2 p_3}{3p_1}\sin\bar\mu_1 c_1\Bigg] + \frac{1}{2}\frac{p_2 p_3}{p_1}c_1\cos\bar\mu_1 c_1 - \frac{1}{2}p_2 c_3\cos\bar\mu_3 c_3\\ &-\frac{1}{2}p_3 c_2\cos\bar\mu_2 c_2\Bigg) + \frac{\ell_o^2}{4}(1+\gamma^2)\Bigg(4p_1 - 2p_1\left(\frac{p_2^2}{p_3^2}+\frac{p_3^2}{p_2^2}\right) + 2\frac{p_2^2 p_3^2}{p_1^3}\Bigg)\Bigg]. \quad (4.66)\end{aligned}$$

The equations for $\dot{p_2}, \dot{p_3}, \dot{c_2}$ and $\dot{c_3}$ are the same modulo the appropriate permutations. Note that it is easy to extend this for other matter fields and also to the vacuum case simply by appropriately modifying the matter part of the effective Hamiltonian constraint.

In the embedding approach these effective equations provide quantum geometry corrections to the classical equations of motion Eqs. (4.18) and (4.19) due to the area gap. However, careful numerical work comparing the full quantum dynamics to the effective dynamics is necessary to determine how accurate the effective equations are.

Now, it is well known that classical Bianchi IX space-times with a massless scalar field as a matter source behave in an asymptotically velocity term dominated (AVTD) manner[7], that is to say that the potential term is negligible (see [92] and references therein). For certain regions of phase space, this will occur *before* quantum gravity effects become important and we will assume that in this case only quantum gravity corrections to the velocity terms are relevant.

It then follows that this behaviour is identical to that of the Bianchi I model and therefore the effective Friedmann equation for the Planck regime to first order in $\hbar$ is given by [81]

$$H^2 = \frac{8\pi G}{3}\rho\left(1-\frac{\rho}{\rho_c}\right) + \frac{\Sigma^2}{6} - \frac{\Sigma^2\rho}{2\rho_c} - \frac{(\Sigma^2)^2}{32\pi G\rho_c} + O(\ell_{\rm Pl}^4), \quad (4.67)$$

[7]This is true so long as the constant of motion p_T^2 is large enough so that the three scale factors are all decreasing as the singularity is approached.

where $\rho_c = 3/8\pi\gamma^2\Delta G\ell_{\rm Pl}^2 \approx 0.41\rho_{\rm Pl}$ (recall that $\Delta = 4\sqrt{3}\pi\gamma$ and $\gamma \approx 0.2375$ due to black hole entropy calculations [17]). The expression for Σ^2 is given by

$$\Sigma^2 = \frac{1}{3\gamma^2 p^3}\Big[(p_1c_1 - p_2c_2)^2 + (p_2c_2 - p_3c_3)^2 + (p_3c_3 - p_1c_1)^2\Big], \tag{4.68}$$

and one can show that $p^3\Sigma^2$ is a constant in the AVTD limit [81].

It is clear that there is a bounce ($H^2 = 0$) when the matter energy density reaches

$$\rho_{\rm bounce} = \frac{1}{2}\left[\rho_c - \frac{3\Sigma^2}{16\pi G} + \sqrt{\left(\rho_c - \frac{3\Sigma^2}{16\pi G}\right)\left(\rho_c - \frac{\Sigma^2}{16\pi G}\right)}\right], \tag{4.69}$$

at which point the energy density and curvature will both decrease and leave the Planck regime and the classical dynamics will once again become a good approximation. It follows that the matter energy density is always bounded above by the critical energy density $\rho_c = 0.41\rho_{\rm Pl}$. This is only an upper bound as the matter density at the bounce depends quite strongly on Σ^2 which is a measure of the strength of the gravitational waves: the stronger the gravitational waves are, the lower $\rho_{\rm bounce}$ will be.

The scenario described above relies on the AVTD behaviour of the Bianchi IX cosmology with a massless scalar field occuring before quantum gravity effects become important. In this case, the true Friedmann equation can then be well approximated by Eq. (4.24) in the classical regime and by Eq. (4.67) in the AVTD limit. However, this scenario *will not* be valid for all regions of phase space, in particular where the scalar field momentum p_T is small enough for the chaotic Mixmaster behaviour to appear.

It has been suggested that, by bounding the strength of the potential terms due to inverse triad effects, quantum gravity effects could play an important role in Bianchi IX dynamics and that the chaotic Mixmaster behaviour would be avoided as a result of this for all types of matter fields [75, 76]. In the effective equations presented above, we have ignored the effect of inverse volume corrections (which for the inverse volume operator used in this chapter are only important for $v < 4$) and have only considered the effect of holonomy corrections. If the chaotic behaviour is to be generically avoided in this effective theory, it will be because the repulsive quantum gravity effects will ensure that the Bianchi IX space-time will not remain in high curvature regions long enough for there to occur a sufficient number of Mixmaster bounces for chaos to appear.

For now, this remains a conjecture and one would have to study the Bianchi IX effective equations of motion more carefully, using both analytic and numerical methods, in order to determine whether the bounce is generic and also to see if chaotic behaviour is avoided or not in the effective theory for small p_T^2.

4.5 Discussion

In this chapter we have studied the improved LQC dynamics for Bianchi IX cosmologies where the matter content is a massless scalar field which is used as a relational time parameter. We have shown that the singularities in the classical theory are resolved by quantum gravity effects in the usual manner in LQC: the singular states decouple from the regular ones under the relational dynamics given by the Hamiltonian constraint operator. Finally, in addition to obtaining a well-defined LQC Hamiltonian constraint operator for Bianchi IX space-times, we also derived some effective equations which provide quantum geometry modifications to the classical equations of motion; these corrections disappear in the limit of the area gap going to zero. Although all of the results presented in this chapter were derived for the particular case of a massless scalar field as the matter field, it will be easy to extend the results presented here for other types of matter fields (as well as the vacuum case) for both the quantum and effective theories.

It is important to point out that all of the tools necessary for the task of deriving the LQC dynamics in Sec. 4.3 for Bianchi IX models were already available. First, the form of $\bar{\mu}_i$ was introduced in the study of Bianchi I models in Chapter 2, as were the variables λ_i which greatly simplify the form of the action of the Hamiltonian constraint operator. The other two necessary ingredients for this work are the connection operator and the inverse triad operators, both of which were introduced for the study of Bianchi II models in Chapter 3. In addition, even the factor-ordering choices necessary in the Hamiltonian constraint operator had already been made. Because of this, it is reasonable to expect that no additional machinery should be necessary in order to complete the study of the loop quantum cosmology of the other Bianchi models of type A.

Recall that in the Bianchi I model there exists a projector which ‘integrates out’ the anisotropic degrees of freedom and gives a wave function which only depends on the isotropic degree of freedom v. It has been shown that the dynamics of such a projected wave function are given by the LQC of flat FLRW space-times [86]. One might expect a similar relation to exist between Bianchi IX cosmologies and closed FLRW models but this is not the case due to the λ_i prefactors that appear in Eqs. (4.60) and (4.62).

However, there do exist other prescriptions which can yield the quantum dynamics of a model’s symmetric sector (in this case, the isotropic sector of Bianchi IX). One such prescription is to consider states which are sharply peaked around the configuration and momentum variables corresponding to a symmetric geometry [103]. In this particular case, this corresponds to studying wave functions which are sharply (but not exactly) peaked around an isotropic geometry, i.e., one where $\lambda_1 = \lambda_2 = (v/2)^{1/3}$. For such a wave function, the action of $\hat{\Theta}$ given in Eq. (4.60) is very closely approximated by that of the $\hat{\Theta}$ obtained for closed FLRW space-times in [46, 47][8] modulo some small errors due to the spread of the wave function. Although this is a nice result, it is not particularly strong as it is expected that the spread of such a wave function will grow with respect to the relational time T. Thus, even if the dynamics of an ‘isotropic’ wave function can be well approximated at some T_1 by the closed FLRW Hamiltonian constraint operator, there is no a priori guarantee that the same will be true at a later T_2. A better understanding of dynamical coherent states in LQC could allow one to resolve this issue and determine whether this relation is preserved by the dynamics or not.

Of course, it is important to allow anisotropies in order to study the entire phase space and in this case the action of the Hamiltonian constraint operator, without any simplifications due to symmetries, is quite complex. Numerical studies will be particularly useful in order to obtain an understanding of how the quantum state of a generic Bianchi IX cosmology evolves with time. Most interesting would be a study of states which are sharply peaked around a semi-classical state at late

[8]There are some minor differences due to the presence of inverse triads operators and different factor-ordering choices due to the presence of λ_1 and λ_2 in addition to v in the Bianchi IX model, but these differences are very small compared to the terms in $\hat{\Theta}$.

times and to then evolve them back in time to see what happens as the curvature increases. Based upon previous experience with isotropic models, one might expect to see one or several bounces as the curvature reaches the Planck scale but careful numerical studies are needed in order to check this.

If the BKL conjecture is correct, a good understanding of the quantum dynamics of Bianchi IX cosmologies will lead to a better comprehension of the behaviour of generic space-times as their curvature reaches the Planck scale. If Bianchi IX models are sufficiently rich in order to understand the approach to such regions, it would appear that no singularities would form since, as shown in Sec. 4.3, an initially nonsingular Bianchi IX wave function must remain nonsingular. It is therefore possible that a careful study of the BKL conjecture at the level of the quantum dynamics could provide a no-singularity theorem, a first step in this direction is provided by [99].

A simpler avenue to study quantum gravity effects in Bianchi IX models would be to study the effective dynamics presented in Sec. 4.4. In isotropic models it turns out that the effective dynamics are surprisingly accurate even in the deep Planck regime: the effective equations accurately predict the quantum trajectory throughout the quantum bounce for sharply peaked wave functions. Because of this, it would be interesting to study the dynamics given by the effective equations for Bianchi IX space-times. However, it is essential to see where the effective equations break down, if they do at all. This could be done by including higher order corrections to the effective equations via the moment expansion method or by comparing the predictions of the effective equations to full numerical solutions of the Hamiltonian constraint operator.

An analysis of the effective equations of motion in the case where the asymptotically velocity term dominated behaviour begins before quantum gravity effects become important shows that there is a bounce when the curvature reaches the Planck scale and that the matter energy density is bounded above by the critical energy density $\rho_c \approx 0.41\rho_{\rm Pl}$. This result relies on the AVTD behaviour and is *not* generic. Therefore, one must also examine other areas in the phase space in order to fully understand the predictions of the effective theory, particularly near Planck scales. As the Mixmaster behaviour appears for small p_T^2 during the approach to the singularity in the classical theory, the effective equations can provide a better understanding of how quantum gravity effects may modify the Mixmaster behaviour as well. In particular it is possible that, as for simpler isotropic models and in AVTD case here, these quantum gravity effects will be repulsive and cause a quantum bounce. This would limit the amount of time that the Mixmaster behaviour occurs and the chaos which arises in the classical theory might be avoided due to the short time span of the Mixmaster dynamics. However, this remains a conjecture and much more work, both analytic and numerical, is needed in order to resolve this question.

Finally, it has been pointed out that the dipole cosmology model can be used in order to study the Bianchi IX model [67]. Although that paper studies the Euclidean theory, it would nonetheless be interesting to compare the model presented there with the one developed in this chapter. In particular, [67] suggests two possible approaches in order to obtain the Hamiltonian constraint operator for their model. Comparing the quantum dynamics resulting from these two possibilities to those derived in this chapter could help determine which of the two approaches is the correct one and hence give some insight into the dipole cosmology models and also spin foam models in general. It is also possible to further probe the relation between the canonical and the covariant approaches to LQG via LQC by extending the Feynman path integral construction given in [60, 61, 62, 64] for the flat FLRW model to the Bianchi IX model; this extension would be nontrivial due to the additional degrees of freedom present in Bianchi IX space-times but it could also improve our understanding of the connection between the canonical and covariant approaches to LQG as well as the relation between full LQG and the symmetry-reduced models of LQC.

Chapter 5

From Bianchi I to the Gowdy Model

5.1 Introduction

When anisotropic models were first studied, there appeared two natural generalizations to the $\bar{\mu}$-scheme, which were presented in [81] (see footnote 1 in Chapter 2 and Sec. 2.3.2 for more details). Since one of these was considerably simpler to work with a lot of the initial LQC work studying Bianchi I models followed this procedure until several problems were pointed out [79, 83, 115]. In particular, the scaling properties of the (more complicated) alternate procedure presented in Chapter 2 have proven to be more suitable [80, 86]. We will refer to these two $\bar{\mu}$-schemes —i.e., the original simpler scheme and the more complicated one recently studied in [86]— as schemes A and B respectively.

The first aim of this chapter is to complete the loop quantization of the vacuum Bianchi I model within scheme B, whose kinematical structure has been established in [86] and later analyzed in detail in [90]. We will see that the Hamiltonian constraint of the model provides a difference equation in an internal discrete parameter v, which is strictly positive and proportional to the volume of the Bianchi I universe. Employing the form of the superselection sectors for the anisotropies determined in [90], we will show here that the quantum evolution equation is indeed well-defined *in vacuo*, namely, that one can use v as a "time" variable and evolve the wave function in terms of it. In other words, we will show that a set of initial data, given on the section of minimum v, completely determines the physical solutions. Owing to this fact, we will be able to obtain the physical structure of the vacuum Bianchi I model for the first time.

An extra motivation for the consideration of the vacuum Bianchi I model with the spatial topology of a three-torus is that its solutions coincide with the subset of homogeneous solutions (the homogeneous sector) of the Gowdy T^3 model with linear polarization [123, 124]. Based on the quantization of vacuum Bianchi I given here, one can then face the quantization of the Gowdy model in the framework of LQC, allowing for the introduction of inhomogeneities.

The Gowdy T^3 model with linear polarization can be viewed as the simplest inhomogeneous cosmological model. These cosmological spacetimes admit two axial Killing vector fields [123, 124] and they describe universes devoid of matter which generically start with an initial curvature singularity [125, 126]. Their quantization by standard methods has been discussed in detail in the literature (see, e.g., [127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137]). It is now well known that after a complete deparametrization, the model admits an essentially unique Fock quantization with certain desired properties [133, 134, 135, 136, 137]. This explains the attention that has already been paid to the quantization of the Gowdy T^3 spacetimes in the framework of the loop theory [84, 85, 138, 139], with the two-fold purpose of including inhomogeneities in LQC and achieving the quantum resolution of the singularities of the model. In particular, [84, 85] succeeded in doing this by proposing a hybrid quantization which combines the loop quantization of the Bianchi type I homogeneous sector —where scheme A was adopted for the improved dynamics— with the natural Fock quantization given in [133, 134, 135, 136, 137] for the inhomogeneities. Since it is generally accepted that scheme A must be replaced with the new scheme B in the quantization of the Bianchi I model, the second goal of this work is to discuss and complete the hybrid quantization of the Gowdy model making use of this alternate scheme for the homogeneous sector. With this aim, we will put on a rigorous basis some steps that are essential for the construction of a well-defined hybrid quantum model and which were left unfinished in [90].

Even though the kinematical Hilbert space of the hybrid procedure is naturally separated as the tensor product of two subspaces, namely the polymer space of the homogeneous sector times the Fock space for the inhomogeneities, the feasibility of this hybrid procedure is not at all trivial. As we will see, the Hamiltonian constraint of the model couples both sectors in a complicated way and it is not obvious whether the constraint can in fact be promoted to a well-defined operator, especially since the inhomogeneous sector contains an infinite number of degrees of freedom. Despite the complexity of the model, it was shown in [84, 85] that indeed the resulting hybrid quantization can be defined properly for scheme A and the corresponding physical Hilbert structure was obtained. Although a priori no relation of this structure with the kinematical one can be presumed, the standard quantum Fock description for the inhomogeneities was recovered in fact at the physical level. Now, the additional difficulties associated with scheme B, where holonomies along different directions no longer commute, make the new problem considerably more complicated. In this chapter, we will prove that the scheme B hybrid quantization of the Gowdy T^3 model is viable.

Let us mention that, apart from the analyses of the Gowdy model, other studies in the literature that have investigated the role of inhomogeneities in the framework of LQC are [66], which adopts a truncation of LQG and employs an approximation of the Born-Oppenheimer type, and the effective analysis of [140, 141].

This chapter is organized as follows. In Sec. 5.2 we recall and summarize the kinematical structure of the vacuum Bianchi I model with T^3 topology in LQC adopting scheme B. In Sec. 5.3, first we prove that the notion of evolution with respect to the volume is well-posed as the associated initial value problem is well-defined, and then we complete the quantization, characterizing the physical Hilbert space and a(n over) complete set of physical observables. In Sec. 5.4, using the results obtained for the Bianchi I model, we show that the quantum dynamics of the Gowdy cosmology is also well-defined when we employ scheme B in its hybrid quantization. Finally, we conclude in Sec. 5.5 with a discussion of our results and further comments.

5.2 Bianchi I T^3 Model in Vacuo: Kinematics

This section summarizes the kinematical structure of the Bianchi I model quantized adopting scheme B for the improved dynamics prescription. We also include the description of the superselection sectors. We refer the reader to [86, 90] for more details.

5.2.1 Vacuum Bianchi I Hamiltonian Constraint

In order to describe the classical model, we choose angular coordinates $\theta, \sigma, \delta \in S^1$ in which the spatial metric is diagonal. The elementary variables in loop quantum gravity are the Ashtekar-Barbero connection and the densitized triad. In the Bianchi I model, owing to homogeneity, each of them can be parametrized in a diagonal gauge by three coefficients. In terms of the fiducial co-triad $\{\mathrm{d}\theta, \mathrm{d}\sigma, \mathrm{d}\delta\}$ and the corresponding densitized fiducial triad, the coefficients of the Ashtekar-Barbero connection are given by $c_i/(2\pi)$ and those of the densitized triad by $p_i/(4\pi^2)$, with $i \in \{\theta, \sigma, \delta\}$ and where the denominators of 2π come from the periods of our coordinates. These coefficients form three pairs of canonical variables, with

$$\{c_i, p_j\} = 8\pi G\gamma\delta_{ij}. \tag{5.1}$$

Here, γ is the Immirzi parameter, G is Newton's constant, and δ_{ij} the Kronecker delta.

For the study of Bianchi I models in LQC using scheme B, it proves useful to introduce the variables

$$\lambda_i = \frac{\mathrm{sgn}(p_i)\sqrt{|p_i|}}{(4\pi\gamma\sqrt{\Delta})^{1/3}\ell_{\mathrm{Pl}}} \quad \text{and} \quad b_i = \sqrt{\left|\frac{p_i \Delta \ell_{\mathrm{Pl}}^2}{p_j p_k}\right|}c_i, \tag{5.2}$$

where $\ell_{\mathrm{Pl}} = \sqrt{G\hbar}$ is the Planck length while the area $\Delta\ell_{\mathrm{Pl}}^2$ is the gap in the spectrum of the area operator in LQG. In these equations, it is understood that repeated indices are not summed over and that the indices i, j, k are all different. Note that the above change of variables is in fact well-defined only for nonvanishing triad variables p_i. Later on, we will see that this suffices for the study of the kinematical arena in LQC.

It is also convenient to introduce the variable

$$v = 2\lambda_\theta\lambda_\sigma\lambda_\delta, \tag{5.3}$$

which is proportional to the physical volume of the Bianchi I universe.

The operators that appear in the Hamiltonian constraint of the Bianchi I model for the considered scheme (see Chapter 2 for details) are $\hat{\lambda}_i$ and $\widehat{\sin b_i}$ (or, equivalently, complex exponentials of b_i). It is easiest to work in the λ_i representation, and in this case $\hat{\lambda}_i$ acts by multiplication while

$$\widehat{e^{ib_\theta}}\Psi(\lambda_\theta, \lambda_\sigma, \lambda_\delta) = \Psi\left(\lambda_\theta - \tfrac{1}{|\lambda_\sigma\lambda_\delta|}, \lambda_\sigma, \lambda_\delta\right), \tag{5.4}$$

and likewise for the other complex exponentials of the b_i's. Finally, it is most convenient to change the configuration variables from $(\lambda_\theta, \lambda_\sigma, \lambda_\delta)$ to, e.g., $(v, \lambda_\sigma, \lambda_\delta)$, since v behaves in a simple manner under the action of $\widehat{e^{ib_i}}$, namely

$$\widehat{e^{ib_\theta}}\Psi(v, \lambda_\sigma, \lambda_\delta) = \Psi\left(v - 2 \cdot \mathrm{sgn}(\lambda_\sigma\lambda_\delta), \lambda_\sigma, \lambda_\delta\right), \tag{5.5}$$

$$\widehat{e^{ib_\sigma}}\Psi(v, \lambda_\sigma, \lambda_\delta) = \Psi\left(v - 2 \cdot \mathrm{sgn}(v\lambda_\sigma), \tfrac{v-2\cdot\mathrm{sgn}(v\lambda_\sigma)}{v} \cdot \lambda_\sigma, \lambda_\delta\right), \tag{5.6}$$

where the symbol sgn denotes the sign function. The action of $\widehat{e^{ib_\delta}}$ is obtained by interchanging the roles of λ_σ and λ_δ in the last equation. Thus, the effect of these holonomy operators on the dependence in v is just a constant shift (up to a sign).

The Hamiltonian constraint operator obtained with a suitable choice of lapse and factor ordering is given in scheme B by

$$\hat{\mathcal{C}}_H = -\frac{1}{16\pi G\gamma^2}\Big[\hat{\Theta}_\theta\hat{\Theta}_\sigma + \hat{\Theta}_\sigma\hat{\Theta}_\theta + \hat{\Theta}_\theta\hat{\Theta}_\delta + \hat{\Theta}_\delta\hat{\Theta}_\theta + \hat{\Theta}_\sigma\hat{\Theta}_\delta + \hat{\Theta}_\delta\hat{\Theta}_\sigma\Big], \tag{5.7}$$

where

$$\hat{\Theta}_i = \pi\gamma\ell_{\mathrm{Pl}}^2\widehat{\sqrt{|v|}}\Big[\widehat{\sin(b_i)}\widehat{\mathrm{sgn}(\lambda_i)} + \widehat{\mathrm{sgn}(\lambda_i)}\widehat{\sin(b_i)}\Big]\widehat{\sqrt{|v|}}. \tag{5.8}$$

Note that this is a different factor ordering choice for $\hat{\Theta}_i$ than what was chosen in the original paper [86], though Chapter 2 has been updated so that it uses this factor ordering as well. This choice is preferable because the operator has the same action on wave functions supported at large values of λ_i while its action for small values of λ_i is much simpler and the consequences are more transparent. Most importantly, the action of this operator does not allow any communication between different $(\lambda_\theta, \lambda_\sigma, \lambda_\delta)$ octants [82, 84, 90].

Under the action of $\hat{\mathcal{C}}_H$, the zero volume states decouple. Therefore, the singularities are resolved kinematically inasmuch as the quantum states that would correspond to them can be removed in practice from the kinematical Hilbert space [82, 84, 90]. Besides, under the action of this Hamiltonian constraint, the different octants remain invariant. Then, each octant contains different superselection sectors. This and the fact that the octants are all related by parity allow us to restrict our attention to the (strictly) positive octant. We do this for the remainder of this chapter. Then, the Hamiltonian constraint acting on a wave function where $v > 4$ gives

$$\begin{aligned}0 =& \sqrt{v}\Big[(v+2)\sqrt{v+4}\,\Psi_4^+(v+4,\lambda_\sigma,\lambda_\delta) - (v+2)\sqrt{v}\,\Psi_0^+(v,\lambda_\sigma,\lambda_\delta)\\ &- (v-2)\sqrt{v}\,\Psi_0^-(v,\lambda_\sigma,\lambda_\delta) + (v-2)\sqrt{v-4}\,\Psi_4^-(v-4,\lambda_\sigma,\lambda_\sigma)\Big].\end{aligned} \tag{5.9}$$

Here $\Psi_{0,4}^\pm$ are defined as follows:

$$\begin{aligned}\Psi_n^\pm(v\pm n,\lambda_\sigma,\lambda_\delta) = \,& \Psi\left(v\pm n, \tfrac{v\pm n}{v\pm 2}\cdot\lambda_\sigma, \tfrac{v\pm 2}{v}\cdot\lambda_\delta\right) + \Psi\left(v\pm n, \tfrac{v\pm n}{v\pm 2}\cdot\lambda_\sigma, \lambda_\delta\right)\\ &+ \Psi\left(v\pm n, \tfrac{v\pm 2}{v}\cdot\lambda_\sigma, \tfrac{v\pm n}{v\pm 2}\cdot\lambda_\delta\right) + \Psi\left(v\pm n, \tfrac{v\pm 2}{v}\cdot\lambda_\sigma, \lambda_\delta\right)\\ &+ \Psi\left(v\pm n, \lambda_\sigma, \tfrac{v\pm 2}{v}\cdot\lambda_\delta\right) + \Psi\left(v\pm n, \lambda_\sigma, \tfrac{v\pm n}{v\pm 2}\cdot\lambda_\delta\right).\end{aligned} \tag{5.10}$$

On the other hand, if $2 < v \leq 4$, the contribution of Ψ_4^- disappears in Eq. (5.9), whereas if $0 < v \leq 2$ the two last contributions in that equation, namely those proportional to Ψ_4^- and Ψ_0^-, are absent.

5.2.2 Superselection Sectors

It was already pointed out in Chapter 2 that there are superselection sectors in v, denoted by a continuous parameter $\epsilon \in (0,4]$. Given such a superselection sector, wave functions only have support on points where $v = \epsilon + 4n$, n being a natural number.

Remarkably, there are also superselection sectors in the λ_i's, although these sectors have a quite different structure compared to those in v. As it is shown in [90], given ϵ and an initial value $\lambda_i^\star > 0$, the wave function will only have support on those points that can be expressed in the form

$$\lambda_i = \left(\frac{\epsilon-2}{\epsilon}\right)^z \prod_k \left(\frac{\epsilon+2m_k}{\epsilon+2n_k}\right)^{p_k} \lambda_i^\star, \tag{5.11}$$

for some k, where m_k, n_k, and p_k are nonnegative integers, and z is any integer unless $\epsilon \leq 2$, in which case $z = 0$. Note that different $\lambda_i^\star$'s will yield the same superselection sector if they are related by Eq. (5.11). It is not difficult to see that one of the available superselection sectors is the set of nonnegative rational numbers (it suffices to consider the case $\epsilon = 0$ with $\lambda_i^\star$ being a rational number). Furthermore, it follows from Eq. (5.11) that each superselection sector is countable, dense in $\mathbb{R}^+$, and that all superselection sectors are isomorphic [90].

Finally, one can show that the form of the superselection sectors for the three wave function variables $(v, \lambda_\sigma, \lambda_\delta)$ is characterized by three numbers $(\epsilon, \lambda_\sigma^\star, \lambda_\delta^\star)$, and is given by the tensor product of the superselection sectors for each individual variable, that is to say that there is no restriction on the sector of λ_δ given that of λ_σ or vice versa [90]. In particular, note that if $\lambda_\sigma^\star$ and $\lambda_\delta^\star$ are compatible in the sense of Eq. (5.11), then the superselection sectors of λ_σ and λ_δ are the same. It is clear that, given one superselection sector $(\epsilon, \lambda_\sigma^\star, \lambda_\delta^\star)$, a wave function will only have support on a countable number of points. Now, whereas the superselection sector in v only contains information about a discrete set of points separated by a constant shift, the superselection sector in the λ_i's encodes the information of a set of points which are densely distributed in the positive quadrant of $(\lambda_\sigma, \lambda_\delta)$.

5.3 Bianchi I T^3 Model in Vacuo: Physical Structure

In this section we will analyze the solutions to the Hamiltonian constraint. We see from Eq. (5.9) that the constraint provides a difference equation in the parameter v, and thus it can be regarded as a (discrete) evolution equation in this parameter. In the analysis of Bianchi I carried out in Chapter 2, a matter content was added, and the notion of evolution was developed in terms of a massless scalar field, instead of doing it in terms of this volume parameter v, which has a purely geometric nature. In the former case, thanks to the suitable properties of the massless field, which is quantized in a standard Schrödinger-like representation, it is straightforward to prove that the associated initial value problem is well posed. In fact, in this respect the situation is quite similar to that found in (relativistic) Quantum Mechanics. Nonetheless, regarding the geometry part, the physical structure of the solutions remained unanswered. Now, in the vacuum case considered here, the role of "time" is played by the volume variable v, which has been polymerically quantized. Because of its discrete nature, the fact that the associated notion of evolution is well-defined is not trivial. We will show in this section that the dynamics are correctly posed: a set of initial data evaluated on the section of initial v completely determines the physical solution. As we will see, the proof is not direct, owing to the complexity of scheme B. In turn, this result will allow us to obtain for the first time the physical Hilbert space of the vacuum Bianchi I model in LQC and a(n over) complete set of observables, thus completing the quantization of the model.

5.3.1 Solutions to the Hamiltonian Constraint

Since we do not expect generic solutions to the Hamiltonian constraint to be normalizable in the kinematical Hilbert space, we will look for solutions in a larger space, namely the algebraic dual of a suitable domain of definition for the Hamiltonian constraint operator. It will be convenient to work with the variables $x_i = \ln \lambda_i$ instead of the λ_i's themselves, as the former variables run over the real line while the latter are positive and, besides, the x_i's suffer displacements under the action of the Hamiltonian constraint operator instead of dilatations or contractions. In fact, from Eq. (5.11), the superselection sectors in x_i are formed by those points such that $(x_i - \ln \lambda_i^\star) = w_i \in \mathcal{Z}_\epsilon$, where

$$\mathcal{Z}_\epsilon = \left\{ z \ln \left(\frac{\epsilon - 2}{\epsilon} \right) + \sum_k \bar{p}_k \ln \left(\frac{\epsilon + 2\bar{m}_k}{\epsilon + 2\bar{n}_k} \right) \right\}. \tag{5.12}$$

Here, for convenience, we have slightly changed the notation with respect to Eq. (5.11), so that now $\bar{m}_k \geq \bar{n}_k$ are nonnegative integers, and $\bar{p}_k$ can take any integer value. Recall that z is any integer unless $\epsilon \leq 2$ in which case $z = 0$. We note that $\mathcal{Z}_\epsilon$ is dense in the real line, because the superselection sectors of λ_i are dense in $\mathbb{R}^+$ and the logarithm is a continuous function from the positive axis to the real line. In spite of the introduction of the x_i's, we will still keep v as one of our variables given its nice behaviour under the action of the Hamiltonian constraint operator.

Since the Wheeler-DeWitt equation associated to the Bianchi I model is actually a first order differential equation in the three variables x_i, it should be possible to determine the entire solution to the Hamiltonian constraint supplying as initial data its restriction to one Cauchy slice (i.e., a surface with constant value of one of the x_i's or alternatively with constant v). However, the constraint in LQC is a second order difference operator for generic values of v. Therefore, it is not immediately clear how the solution can be determined from one slice of initial data obtained at a constant value of v. The solution lies in the different form that the action of the Hamiltonian constraint operator has on states with $v \leq 4$, this form is that of a first order difference equation.

Given a superselection sector in v, denoted by $\epsilon \in (0, 4]$, one obtains this first order difference equation in v for $v = \epsilon + 4$ in terms of the initial data on the slice $v = \epsilon$. If one can solve this (highly coupled) difference equation, it will then be possible to solve the (again highly coupled) second order difference equation for $v = \epsilon + 8$ in terms of the data on the slices $v = \epsilon$ and $v = \epsilon + 4$. One can then follow this strategy in order to obtain the full solution to the Hamiltonian constraint for all v. Finally, because the $v + 4$ terms always appear in the same combination, given by Ψ_4^+, we only need to show how to derive the data on $v = \epsilon + 4$, and then the data for all other v can be obtained in the same manner.

The difference equation we are interested in is

$$\Psi_4^+(\epsilon + 4, x_\sigma, x_\delta) = \sqrt{\frac{\epsilon}{\epsilon + 4}} \Big[\Psi_0^+(\epsilon, x_\sigma, x_\delta) + \frac{\epsilon - 2}{\epsilon + 2} \theta_{\epsilon-2} \Psi_0^-(\epsilon, x_\sigma, x_\delta) \Big]. \tag{5.13}$$

Since the righthand side is known, the question is just whether one is able to obtain $\Psi(\epsilon + 4, x_\sigma, x_\delta)$ from $\Psi_4^+(\epsilon + 4, x_\sigma, x_\delta)$ in order to derive the form of the wave function for all v.

The explicit form of Ψ_4^+ is given by:

$$\begin{aligned} \Psi_4^+(v + 4, x_\sigma, x_\delta) = & \, \Psi\left(v + 4, x_\sigma, \ln\left(\tfrac{v+4}{v+2}\right) + x_\delta\right) + \Psi\left(v + 4, \ln\left(\tfrac{v+4}{v+2}\right) + x_\sigma, x_\delta\right) \\ & + \Psi\left(v + 4, x_\sigma, \ln\left(\tfrac{v+2}{v}\right) + x_\delta\right) + \Psi\left(v + 4, \ln\left(\tfrac{v+2}{v}\right) + x_\sigma, x_\delta\right) \\ & + \Psi\left(v + 4, \ln\left(\tfrac{v+2}{v}\right) + x_\sigma, \ln\left(\tfrac{v+4}{v+2}\right) + x_\delta\right) \\ & + \Psi\left(v + 4, \ln\left(\tfrac{v+4}{v+2}\right) + x_\sigma, \ln\left(\tfrac{v+2}{v}\right) + x_\delta\right) \end{aligned} \tag{5.14}$$

for any value of v (and, in particular, for $v = \epsilon$). It can be expressed as the result of the action of two separate operators,

$$\Psi_4^+(v+4, x_\sigma, x_\delta) = \hat{U}_6(v+4)\hat{A}\Psi(v, x_\sigma, x_\delta), \tag{5.15}$$

where $\hat{A}$ only shifts the value of v, namely,

$$\hat{A}\Psi(v, x_\sigma, x_\delta) = \left(\widehat{e^{-ib_\theta}}\right)^2 \Psi(v, x_\sigma, x_\delta) = \Psi(v+4, x_\sigma, x_\delta), \tag{5.16}$$

while

$$\begin{aligned}\hat{U}_6(v)\Psi(v, x_\sigma, x_\delta) = \Big[&\widehat{e^{-ib_\theta}}\widehat{e^{-ib_\sigma}} + \widehat{e^{-ib_\sigma}}\widehat{e^{-ib_\theta}} + \widehat{e^{-ib_\sigma}}\widehat{e^{-ib_\delta}} + \widehat{e^{-ib_\delta}}\widehat{e^{-ib_\sigma}} \\ &+ \widehat{e^{-ib_\delta}}\widehat{e^{-ib_\theta}} + \widehat{e^{-ib_\theta}}\widehat{e^{-ib_\delta}}\Big]\left(\widehat{e^{ib_\theta}}\right)^2 \Psi(v, x_\sigma, x_\delta)\end{aligned} \tag{5.17}$$

has a trivial action on the v-sector.

The invertibility of the operator $\hat{U}_6(v)$ for any value of v would guarantee that one can determine $\Psi(v, x_\sigma, x_\delta)$ from $\Psi_4^+(v, x_\sigma, x_\delta)$. Assuming for the moment that the inverse operator $[\hat{U}_6(v)]^{-1}$ exists, we can derive the state at the volume $\epsilon + 4$ by calculating

$$\Psi(\epsilon+4, x_\sigma, x_\delta) = \sqrt{\frac{\epsilon}{\epsilon+4}}\Big[\hat{U}_6(\epsilon+4)\Big]^{-1}\Big[\Psi_0^+(\epsilon, x_\sigma, x_\delta) + \frac{\epsilon-2}{\epsilon+2}\Psi_0^-(\epsilon, x_\sigma, x_\delta)\Big]. \tag{5.18}$$

Once again, the second term in the square brackets on the right hand side of this equation does not appear if $\epsilon \leq 2$.

Again assuming the existence of $[\hat{U}_6(v)]^{-1}$, it is now straightforward to obtain the value of the wave function for the section $v = \epsilon + 8$:

$$\begin{aligned}\Psi(\epsilon+8, x_\sigma, x_\delta) =& \sqrt{\frac{\epsilon+4}{\epsilon+8}}\Big[\hat{U}_6(\epsilon+8)\Big]^{-1}\Bigg[\Psi_0^+(\epsilon+4, x_\sigma, x_\delta) + \frac{\epsilon+2}{\epsilon+6}\Psi_0^-(\epsilon+4, x_\sigma, x_\delta) \\ &- \frac{\epsilon+2}{\epsilon+6}\sqrt{\frac{\epsilon}{\epsilon+4}}\,\Psi_4^-(\epsilon, x_\sigma, x_\delta)\Bigg].\end{aligned} \tag{5.19}$$

It is clear how to repeat this procedure in order to get the value of the wave function for all larger v as well. Therefore, if the operator $\hat{U}_6(v)$ can be inverted we conclude that the initial value problem in terms of v is well posed, at least at $v = \epsilon$. In the next section we show that indeed this is the case.

5.3.2 The Operator $\hat{U}_6$

Let us then analyze the operator $\hat{U}_6(v)$ to see that its action can be inverted. First, we provide a suitable domain of definition for $\hat{U}_6(v)$, keeping fixed the value of v (in other words, we restrict the discussion just to a slice of constant v). For each direction $i = \sigma$ or δ, consider the linear span $\mathrm{Cyl}_{\lambda_i^\star}$ of the states whose support is just one point x_i of the superselection sector determined by Eq. (5.12), with $(x_i - \ln \lambda_i{}^\star) = w_i \in \mathcal{Z}_\epsilon$. We call $\mathcal{H}_{\lambda_i^\star}$ the Hilbert completion of this vector space with the discrete inner product. Then, we can choose the tensor product $\mathrm{Cyl}_{\lambda_\sigma^\star} \otimes \mathrm{Cyl}_{\lambda_\delta^\star}$ as the domain for $\hat{U}_6(v)$.

Now, if we define on the Hilbert space $\mathcal{H}_{\lambda_\sigma^\star} \otimes \mathcal{H}_{\lambda_\delta^\star}$ the translations

$$\hat{U}^{(w_\sigma, w_\delta)} \Psi(v, x_\sigma, x_\delta) = \Psi(v, w_\sigma + x_\sigma, w_\delta + x_\delta), \tag{5.20}$$

then the operator $\hat{U}_6(v)$ is just a sum of six translations of this kind. These translation operators are unitary because, if w_σ and w_δ are two numbers in $\mathcal{Z}_\epsilon$, so that a shift of x_i by any of them leaves invariant the superselection sector [see Eq. (5.12)], then the sum of $|\hat{U}^{(w_\sigma, w_\delta)} \Psi(v, x_\sigma, x_\delta)|^2$ over all x_σ and x_δ in the superselection sector coincides with the sum of $|\Psi(v, x_\sigma, x_\delta)|^2$. Moreover, owing to this property and the Schwarz inequality, we conclude that the norm of the operator $\hat{U}_6(v)$ is bounded by 6.

Since $\hat{U}_6(v)$ is bounded, it can be extended as a well-defined operator to the entire Hilbert space. This extension [which we also denote by $\hat{U}_6(v)$] provides in fact a normal operator —namely, the operator commutes with its adjoint— as the translations in x_σ and/or in x_δ commute. Hence, in particular, it is guaranteed that the residual spectrum is empty. Thus the operator $\hat{U}_6(v)$ is invertible in our Hilbert space if and only if its point spectrum does not contain the zero.

It is not difficult to convince oneself that the point spectrum of $\hat{U}_6(v)$ must be empty owing to the properties of the operator. The idea is that since this operator is just a linear combination of translations, any of its eigenfunctions must possess a certain translational invariance which would prevent them from being normalizable. In order to see this, let us consider again the translations $\hat{U}^{(w_\sigma,w_\delta)}$, with $w_\sigma, w_\delta \in \mathcal{Z}_\epsilon$. Since they all commute with each other as well as with $\hat{U}_6(v)$, they can all be diagonalized simultaneously, that is, there exists a basis of common (generalized) eigenfunctions. Let us call in the following

$$\hat{U}_\sigma^{w_\sigma} = \hat{U}^{(w_\sigma,0)}, \quad \hat{U}_\delta^{w_\delta} = \hat{U}^{(0,w_\delta)}, \tag{5.21}$$

so that $\hat{U}^{(w_\sigma,w_\delta)} = \hat{U}_\sigma^{w_\sigma}\hat{U}_\delta^{w_\delta}$. Given one of the eigenfunctions common to all of these translations, we denote the corresponding eigenvalue of $\hat{U}_i^{w_i}$ by $\rho_i(w_i)$ (with $i = \sigma, \delta$). This eigenvalue must be a complex number of unit norm, because the translation operators are unitary. In addition, since $\hat{U}_i^{w_i}\hat{U}_i^{\bar{w}_i} = \hat{U}_i^{w_i+\bar{w}_i}$, it follows that

$$\rho_i(w_i)\rho_i(\bar{w}_i) = \rho_i(w_i + \bar{w}_i). \tag{5.22}$$

Recalling that all points in the superselection sector can be reached from $\ln \lambda_i^\star$ by a translation $\hat{U}_i^{w_i}$, it is a simple exercise to show that the eigenfunctions are proportional to $\rho_\sigma(w_\sigma)\rho_\delta(w_\delta)$. We can always change this wave function by a constant of unit norm, and thus we fix $\rho_i(0) = 1$. Besides, in order to determine completely the wave function, we only need to know the value of $\rho_i(w_i)$ in an appropriate subset of $\mathcal{Z}_\epsilon$, namely any collection of noncommensurable points which can generate the entire set by multiplication by integers. It is possible to see that the property in Eq. (5.22) provides then all the information about ρ_i at the rest of points in $\mathcal{Z}_\epsilon$. In particular, $\rho_i(nw_i) = [\rho_i(w_i)]^n$.

The wave functions $\rho_i(w_i)$ are clearly nonnormalizable with respect to the discrete inner product in $\mathcal{H}_{\lambda_i^\star}$ as they have complex unit norm at each point of the superselection sector (the shift of $\mathcal{Z}_\epsilon$ by $\ln \lambda_i^\star$) and the sector contains an infinite number of points. In addition, different wave functions $\rho_i(w_i)$ must be orthogonal, because there always exists a (unitary) translation operator on $\mathcal{H}_{\lambda_i^\star}$ whose eigenvalue differs for the two wave functions.

At this stage of the discussion, it is worth noticing that, by the very construction of the algebra of fundamental operators in LQC previous to the introduction of superselection sectors, the operators $\hat{U}_i^{w_i}$ that act as translations in the x_i representation can be identified in the holonomy/connection representation —where they act as multiplicative operators— as elements of the Bohr compactification of the real line, $\mathbb{R}_{\text{Bohr}}$ [142]. These elements can be understood as maps ρ_i from the real line (corresponding to all possible real values of x_i, or equivalently of w_i) to the circle such that they satisfy condition (5.22) and $\rho_i(0) = 1$. Owing to superselection, however, the values of w_i are now restricted to belong to $\mathcal{Z}_\epsilon$. We can then identify the wave functions $\rho_i(w_i)$ as equivalence classes of elements in $\mathbb{R}_{\text{Bohr}}$, the equivalence relation being the identification of all those maps ρ_i which differ only by their action on the set complementary to $\mathcal{Z}_\epsilon$ in the real line, i.e., $\mathbb{R} \setminus \mathcal{Z}_\epsilon$. Examples of $\rho_i(w_i)$ are provided by the exponential maps $\exp(ik_i w_i)$ from $\mathcal{Z}_\epsilon$ to S^1. Since $\mathcal{Z}_\epsilon$ contains noncommensurable numbers, these exponentials separate all real values of k_i [that is, for any two values of k_i one can find a value of w_i for which the exponentials $\exp(ik_i w_i)$ are different]. So, the set of possible and distinct ρ_i contains all the exponentials with $k_i \in \mathbb{R}$.

Returning to the operator $\hat{U}_6(v)$, it is straightforward to find its eigenvalue for each of the analyzed wave functions. It is given by

$$\begin{aligned} \omega_6(\rho_\sigma, \rho_\delta) = & \sum_{i=\sigma,\delta} \left\{ \rho_i \left[\ln\left(\tfrac{v}{v-2}\right) \right] + \rho_i \left[\ln\left(\tfrac{v-2}{v-4}\right) \right] \right\} \\ & + \sum_{i,j=\sigma,\delta; i \neq j} \left\{ \rho_i \left[\ln\left(\tfrac{v}{v-2}\right) \right] \rho_j \left[\ln\left(\tfrac{v-2}{v-4}\right) \right] \right\}. \end{aligned} \tag{5.23}$$

Remember that here $v > 4$. The point spectrum of $\hat{U}_6(v)$ will not contain the zero provided that there is no normalizable linear superposition of the above wave functions with $\omega_6(\rho_\sigma, \rho_\delta) = 0$. In this superposition, the measure for ρ_i is continuous: this is a consequence of the wave functions $\rho_i(w_i)$ not being normalizable in $\mathcal{H}_{\lambda_i^\star}$. The restriction to the kernel of $\hat{U}_6(v)$ is achieved then by introducing a delta function of $\omega_6(\rho_\sigma, \rho_\delta)$ (peaked at zero). If one computes the norm of this superposition, the orthogonality of the wave functions $\rho_i(w_i)$ leads to integrals over the square complex norm of each $(\rho_\sigma, \rho_\delta)$-contribution. But this contains a square delta, so that the norm diverges. Therefore, the point spectrum of the operator $\hat{U}_6(v)$ does not contain the zero, as we wanted to show. It is also possible to apply the same line of reasoning for any other possible eigenvalue of $\hat{U}_6$, not just for zero, showing that the point spectrum of this operator is empty.

5.3.3 Physical Hilbert Space

Now that we have seen that the solutions to the Hamiltonian constraint are completely determined by the data on the initial slice $v = \epsilon$, we can identify these solutions with the corresponding initial data and characterize the physical Hilbert space by providing a Hilbert structure to the data, belonging in principle to the dual of the vector space $\text{Cyl}_{\lambda^\star_\sigma} \otimes \text{Cyl}_{\lambda^\star_\delta} \subset \mathcal{H}_{\lambda^\star_\sigma} \otimes \mathcal{H}_{\lambda^\star_\delta}$.

In order to endow them with an inner product, we take a(n over) complete set of classical observables forming a closed algebra, and we impose that the quantum counterpart of their complex conjugation relations become adjointness relations between operators. Such a set is formed by the operators $\widehat{e^{ix_i}}$ and $\hat{U}_i^{\omega_i}$, with $\omega_i \in \mathcal{Z}_\epsilon$ and $i = \sigma, \delta$. For $\psi(\lambda_\sigma, \lambda_\delta) \in \text{Cyl}_{\lambda^\star_\sigma} \otimes \text{Cyl}_{\lambda^\star_\delta}$ (and for the initial data by duality), these operators are defined as

$$\widehat{e^{ix_\sigma}}\psi(x_\sigma, x_\delta) = e^{ix_\sigma}\psi(x_\sigma, x_\delta), \tag{5.24}$$

$$\hat{U}_\sigma^{\omega_\sigma}\psi(x_\sigma, x_\delta) = \psi(x_\sigma + \omega_\sigma, x_\delta), \tag{5.25}$$

and similarly for $\widehat{e^{ix_\delta}}$ and $\hat{U}_\delta^{\omega_\delta}$. Clearly, all these operators are unitary in $\mathcal{H}_{\lambda^\star_\sigma} \otimes \mathcal{H}_{\lambda^\star_\delta}$, according with their reality conditions. Therefore, we conclude that this Hilbert space is precisely the physical Hilbert space of the vacuum Bianchi I model.

5.4 Hybrid Quantization of the Gowdy T^3 Cosmologies

The Gowdy T^3 model can be viewed as homogeneous Bianchi I backgrounds which allow certain inhomogeneous modes of the gravitational field to propagate along one direction. This natural separation in homogeneous and inhomogeneous sectors motivated a hybrid quantization of the model which combines the loop quantization of the Bianchi I phase space with a natural Fock quantization for the inhomogeneities, and which was carried out in [84, 85] adopting scheme A for the improved dynamics in the quantization of the Bianchi I sector. This separation of degrees of freedom is nonperturbative and independent of the strength of the inhomogeneities at the classical level. Although ideally one should perform a LQC quantization for the inhomogeneous degrees of freedom as well, this hybrid approach is justified if the most relevant quantum geometry effects (but not necessarily *all* quantum effects) are those that affect the homogenous background so that one can establish a kind of perturbative hierarchy in their treatment. In addition, it is natural to adopt a Fock quantization of the inhomogeneities in this context based on the expectation that a conventional Fock description of the inhomogeneities ought to be recovered from LQC in a regime where quantum geometry phenomena are negligible. In this case there exists a privileged Fock quantization under certain requirements on the symmetries of the vacuum and on the existence of a unitary dynamics with respect to an emergent time [133, 134, 135, 136, 137]; these properties provide a natural Fock quantization for the inhomogeneous modes.

Here, we will show that the hybrid quantization of the Gowdy model employing scheme B for the loop quantization of the homogeneous sector is also viable. As in previous works with the other scheme [84, 85], this is not a trivial issue owing to the coupling between the homogeneous and inhomogeneous sectors in the Hamiltonian constraint. Moreover, now the structure of the homogeneous sector is much more complicated, owing to the intricacy of the holonomy operators in the new scheme B. The results obtained in Sec. 5.3 will be essential in order to see that the hybrid quantization is well-defined within scheme B as well. Our demonstration provides a necessary justification for the steps followed in [90] where the physical Hilbert space of this new hybrid Gowdy model was obtained.

5.4.1 Kinematical Structure and Hamiltonian Constraint Operator

As in the Bianchi I model studied in Sec. 5.2, since the spatial topology is that of a three-torus, we have $\theta, \sigma, \delta \in S^1$ with a coordinate length of 2π. Following a careful gauge-fixing [85, 143], one finds that the information about the homogeneous degrees of freedom (which describe the subfamily of homogeneous space-times in the Gowdy model) can be encoded in the Bianchi I variables c_i and p_i introduced in Sec. 5.2.1. On the other hand, the inhomogeneities corresponding to the content of gravitational waves can be described by a single metric field (without a zero mode), which in turn can be described by creation and annihilation-like variables

$\{(a_m, a_m^*),\ m \in \mathbb{Z} - \{0\}\}$, defined in the same way as the natural variables that one would adopt if the field behaved as a free massless scalar field. Owing to the partial gauge-fixing, only two global constraints remain on the system: the zero mode of the Hamiltonian constraint, which generates time reparametrizations, and the zero mode of the θ-diffeomorphism constraint, which generates translations around the θ-circle (see [85] for details).

In order to proceed with the hybrid quantization of the Gowdy model, we follow the LQC approach for the homogeneous degrees of freedom and, as in the Bianchi I model, we adopt the prescription $p_i c_i \to \hat{\Theta}_i$ where the operators $\hat{\Theta}_i$ are defined in Eq. (5.8) while for the inhomogeneities we promote the creation and annihilation variables to operators in the standard quantum field theory fashion. The kinematical Hilbert space is then the tensor product of the polymer space of the Bianchi I model times the resulting Fock space for the inhomogeneities [90].

The generator of translations around the θ-circle only affects the inhomogeneities and it is straightforward to impose in the quantum theory [84, 85, 90]. On the other hand, as we pointed out earlier, the Hamiltonian constraint couples the homogeneous and inhomogeneous sectors in a nontrivial way. The resulting operator has the explicit form [90]

$$\begin{aligned}\hat{\mathcal{C}}_H = &-\frac{1}{16\pi G\gamma^2}\left[\hat{\Theta}_\theta\hat{\Theta}_\sigma + \hat{\Theta}_\sigma\hat{\Theta}_\theta + \hat{\Theta}_\theta\hat{\Theta}_\delta + \hat{\Theta}_\delta\hat{\Theta}_\theta + \hat{\Theta}_\sigma\hat{\Theta}_\delta + \hat{\Theta}_\delta\hat{\Theta}_\sigma\right]\\ &+\frac{1}{16\pi}\left(\left[\widehat{\frac{1}{|p_\theta|^{1/4}}}\right]^2 \frac{(\hat{\Theta}_\sigma + \hat{\Theta}_\delta)^2}{\gamma^2}\left[\widehat{\frac{1}{|p_\theta|^{1/4}}}\right]^2 \widehat{\mathcal{H}_{\text{int}}} + 32\pi^2\widehat{|p_\theta|}\widehat{\mathcal{H}_{\text{o}}}\right), \qquad (5.26)\end{aligned}$$

where

$$\widehat{\mathcal{H}_{\text{o}}} = \sum_{m\neq 0}|m|\hat{a}_m^\dagger\hat{a}_m, \qquad \text{and} \qquad (5.27)$$

$$\widehat{\mathcal{H}_{\text{int}}} = \sum_{m\neq 0}\frac{1}{2|m|}\Big(2\hat{a}_m^\dagger\hat{a}_m + \hat{a}_m\hat{a}_{-m} + \hat{a}_m^\dagger\hat{a}_{-m}^\dagger\Big), \qquad (5.28)$$

are the terms that involve the inhomogeneities and the regulated “inverse triad” operator representing $|p_\theta|^{-1/4}$ is given by [87, 90]

$$\left[\widehat{\frac{1}{|p_\theta|^{1/4}}}\right]|v,\lambda_\sigma,\lambda_\delta\rangle = \frac{\sqrt{2|\lambda_\sigma\lambda_\delta|}}{(4\pi\gamma\sqrt{\Delta}\ell_{\mathrm{Pl}}^3)^{1/6}}\Big(\sqrt{|v+1|}-\sqrt{|v-1|}\Big)|v,\lambda_\sigma,\lambda_\delta\rangle. \quad (5.29)$$

Note that Eq. (5.27) is the Hamiltonian of a free massless scalar field and Eq. (5.28) is a quadratic interaction Hamiltonian. Owing to the coupling between these terms and those of the homogeneous sector, *it is not guaranteed that the hybrid approach is physically feasible beyond the kinematical level,* namely, once the constraints are imposed. In the remainder of this section we confirm that one attains in fact a well-defined physical theory.

The explicit form of the action of the Hamiltonian constraint operator on kinematical states is easy to compute as most of the terms in the operator have already been considered in the Bianchi I model or are extensions of well-known operators. The most significant subtleties concern the action of $\widehat{\mathcal{H}_{\mathrm{int}}}$ as this operator includes the sum of all $\hat{a}^\dagger_m\hat{a}^\dagger_{-m}$ terms ($m\neq 0$), each of which creates an extra pair of "particles" in the modes m and $-m$. However, in spite of the fact that $\widehat{\mathcal{H}_{\mathrm{int}}}$ creates an infinite number of particles, one can prove that it is a well-defined operator in a suitable dense domain of the Fock space [90]. On the other hand, it is straightforward to see that $\hat{\mathcal{C}}_H$ leaves invariant Hilbert subspaces which are the tensor product of the superselection sectors of the Bianchi I model times the Fock space. Therefore, as in the Bianchi I model, we can restrict the study to separable Hilbert subspaces whose states have, in the homogeneous sector, quantum numbers $(v,\lambda_\sigma,\lambda_\delta)$ with support in discrete sets contained in the positive octant. Let us remember that while v takes values in a semi-lattice of constant step equal to 4 with a minimum equal to $\epsilon\in(0,4]$, the values of $(\lambda_\sigma,\lambda_\delta)$ densely cover the positive quadrant of the real plane.

Even though, from a physical perspective, one is only interested in small inhomogeneities which produce a perturbation around the homogeneous Bianchi I background, the hybrid quantum model is well-defined and consistent without restrictions on the wave numbers or occupation numbers of the modes, and the evolution can be obtained in much the same manner as in the vacuum Bianchi I model. Using the result that the Bianchi I model in scheme B leads to a well posed initial value problem on the section of constant volume $v=\epsilon$ from which one can evolve the physical state in steps of four units in v, one can show that the physical evolution in the hybrid Gowdy model is also (formally) solvable adopting a perturbative approach, in which the effect of the interaction term $\widehat{\mathcal{H}_{\rm int}}$ is treated as small compared to the free Hamiltonian term $\widehat{\mathcal{H}_{\rm o}}$. Starting with initial data at $v = \epsilon$, one can then find the form of the physical wave functions at $v = \epsilon + 4$ in a perturbative expansion. With this data, one can continue the evolution to the next section $v = \epsilon + 8$. This procedure can be repeated until one obtains the expression of the physical wave function at the wanted value of v and up to the desired perturbative order. Actually, this perturbative expansion can be understood as an asymptotic expansion in the limit in which the Immirzi parameter tends to infinity. The details of this perturbative expansion are presented in [90].

The important point here is that the evolution is well-defined in this perturbative approach. This is mainly due to the fact that the initial value problem for the vacuum Bianchi I sector is well-posed and therefore this result depends upon the proof presented in Sec. 5.3. In this sense, the initial value problems in the vacuum Bianchi I model and the Gowdy T^3 model are closely related.

5.5 Discussion

In this chapter we first considered vacuum Bianchi I universes with a three-torus topology in the framework of LQC, adopting a new scheme for the improved dynamics which was put forward in [86]. We have examined some of the aspects of this quantization which had remained unanswered in [86], like the decoupling of triad components with different orientations under the action of the Hamiltonian constraint, the structure of the superselection sectors in the anisotropies, and the evolution of physical states in terms of the volume as a discrete, internal evolution variable. Then, we showed that the initial value problem is well posed and completed the quantization of the vacuum Bianchi I model, following scheme B for the implementation of the improved dynamics.

In Sec. 5.4, we have used the results regarding the vacuum Bianchi I model in order to show that the scheme B hybrid quantization of the linearly polarized Gowdy T^3 cosmological model is viable. This hybrid quantization provides a first step toward a better understanding of the effect of inhomogeneities in LQC; this is necessary if one wants to eventually obtain predictions about the influence and possible traces of quantum gravity in phenomena like primordial gravitational waves, the cosmic microwave background, and the physics of the early universe in general.

The loop quantization of the Bianchi I model leads to superselection in separable sectors not only for the volume, but also for the anisotropies. Moreover, every superselection sector is restricted to an octant. This is because the Hamiltonian constraint operator, due to appropriate factor ordering choices, does not mix eigenstates of the densitized triad components with different orientations. Moreover, while the superselection sectors in the volume of the Bianchi I universes consist of equidistant points forming a semi-lattice, the superselection sectors in the anisotropies are dense sets in the real semi-axis. On the other hand, the restriction to a definite orientation of the triad components without imposing any kind of boundary conditions, together with the fact that the initial value problem for the evolution is well posed at the minimum value of v (i.e., $v = \epsilon$), can be regarded as a realization of a no-boundary prescription for the dynamics. In addition, it is worth emphasizing the result that the discrete evolution in v is well-defined starting from the initial section $v = \epsilon$. If this were not the case, the evolution would break down for Bianchi I cosmologies in vacuo for scheme B and, without any reasonable justification, the inclusion of matter would turn out to be critical in order for the dynamics of the model to be viable; we have shown that this is not the case.

Concerning the hybrid quantization of the Gowdy model, an important point is that the LQC/Fock split that we have considered assumes that the quantum behaviour of the inhomogeneities can be well approximated by conventional quantum field theory methods so that any quantum geometry effects due to the presence of these inhomogeneities can be neglected as perturbatively small. In a true loop quantization of all the gravitational degrees of freedom (i.e., presumably in a reduction of LQG by a suitable incorporation of the symmetries of the Gowdy model), one should treat both the homogeneous and the inhomogeneous sectors in the same manner, that is to say, all of the degrees of freedom should be quantized à la loop. From this perspective, the main assumption in our analysis is that the qualitative results of the hybrid quantization capture the physics of a full loop quantization so long as the inhomogeneities are not directly affected in a significant way by quantum geometry phenomena. It is worth noticing that similar assumptions are implicit in the treatment of other models with matter in LQC inasmuch as matter fields are usually quantized by standard methods rather than by adopting a unified polymer quantization for all of the degrees of freedom, gravitational or not.

Notice nonetheless that, even at this level, one can see that the hybrid quantization approach is sufficient to ensure that the classical cosmological singularities are resolved as the singular states corresponding to vanishing Bianchi I scale factors decouple under the action of the Hamiltonian constraint operator [90]. In addition, the quantum dynamics are well posed as one can use v as an evolution variable and, given the wave function at $v = \epsilon$, one can derive the wave function for all other values of v in the same superselection sector in a perturbative expansion in the interaction term for the inhomogeneities.

There remain many open questions to be addressed, of course, the most important being a numerical study of the evolution of the wave function. This is a very difficult task as even the vacuum Bianchi I model in LQC has not yet been studied numerically in scheme B. We propose to begin with a simpler task and study effective equations associated to the model; this should yield some insight into the most relevant quantum geometry corrections to the classical model [144]. The most important point, however, is to understand inhomogeneities in LQC more deeply and to do this one will have to consider more general inhomogeneous space-times within the framework of LQC in order to obtain physical predictions about our early universe and understand their consequences.

Chapter 6

Summary and Outlook

In this dissertation we have extended the improved dynamics of loop quantum cosmology to space-times that allow anisotropies and inhomogeneities. The first step was to study the spatially flat Bianchi I model, where it was necessary to determine the correct generalization of the $\bar{\mu}$ scheme to the case where there are three independent scale factors. We then considered two spatially curved homogeneous space-times, the Bianchi type II and type IX models, where a field strength operator could not be introduced due to the presence of both anisotropies and curvature, so we constructed a connection operator instead. This connection operator turns out to be very useful as it can be used in order to complete the missing steps of the loop quantization of the open FLRW model, and it also provides an alternate loop quantization of the closed FLRW model which is presented in Appendix B. Finally, we obtained a hybrid quantization of the linearly polarized Gowdy T^3 model by combining the loop quantization of the Bianchi I background with a Fock quantization of the gravitational wave modes.

The goal of this dissertation was to go beyond the simplest homogeneous and isotropic cosmological models that were first studied in LQC in order to be able to study more realistic models of the universe in which we live as well as testing the robustness of the theory by relaxing some of the symmetries of the simpler models. Although the programme is not yet complete since we do not yet know how to properly describe cosmological space-times which allow arbitrary inhomogeneities within the framework of loop quantum cosmology, the results obtained here represent an important step toward that ultimate goal.

One important result is that the resolution of the classical singularity due to quantum gravity effects appears to be generic. In the Bianchi models as well as the Gowdy model, singular states decouple from nonsingular ones under the dynamics of the theory. In other words, *a nonsingular state will remain nonsingular* throughout its evolution. This is an important check upon the robustness of the results of the isotropic models and indicates that it may be possible to generalize many of the results obtained in simpler models.

However, in order to learn more about the loop quantum cosmology of the Bianchi models as well as the hybrid Gowdy model, it is necessary to perform detailed numerical simulations of the dynamics. In particular, a numerical study of the dynamics of states sharply peaked around classical solutions to Einstein's equations as they are evolved toward high curvature regimes would be very enlightening. In the simple isotropic models, the wave function remained sharply peaked throughout its evolution (with respect to the relational time given by the massless scalar field) and there was a quantum "big bounce" when the matter energy density reached the critical density $\rho_c \approx 0.41\rho_{\rm Pl}$. In addition, it turned out that the evolution of the expectation values of the sharply peaked wave function were very well approximated by an effective equation. For example, for the spatially flat case the effective equation is simply

$$H^2 = \frac{8\pi G}{3}\rho\left(1 - \frac{\rho}{\rho_c}\right). \tag{6.1}$$

When the matter energy density approaches the critical density, quantum gravity effects provide a repulsive force which causes the "big bounce" and hence the avoidance of the classical singularity. It is an open question whether, in the more complicated Bianchi and Gowdy models, the "big bounce" still occurs and also whether the effective equations are as reliable as in the isotropic case. Numerical simulations are necessary in order to answer these questions.

By considering more complex space-times in LQC, we have also had to better understand the relation between LQG and LQC, especially in order to determine which choice of $\bar{\mu}_i$ is the appropriate one. We are still some way from a derivation of LQC from LQG; however, we have seen that by allowing more degrees of freedom in LQC the relation between the two theories becomes clearer. Hopefully, once we move beyond the hybrid quantization of the Gowdy model to a full loop quantization of inhomogeneous space-times, this relation will be even better understood and this will perhaps allow one to derive LQC from LQG.

In addition, we saw how various ambiguities arise during the loop quantization of these space-times, including the choice of $\bar{\mu}_i$, the definition of the connection operator, the definition of the inverse triad operators, and the choice of the parity properties of c_i and p_i. Despite these ambiguities not being the same as those in the full theory, we believe that learning to deal with ambiguities in a simpler setting will be helpful for the more complicated full theory, as it may give some insight into the consequences of some choices.

The next step is to consider space-times that allow more generic inhomogeneities than in the Gowdy model. The Gowdy model has been very useful as a first step because the inhomogeneities are of such a specific type that they are easy to address. However, this also limits the utility of the model since the inhomogeneities in our universe do not resemble those of the Gowdy model; therefore, it is important to continue to study cosmological models that are increasingly realistic. Another goal is to move beyond a hybrid quantization. Although the hybrid quantization is comparatively easy to obtain and we expect it to offer a good approximation in many regimes of physical interest, it is very important to understand how to obtain the full loop quantum cosmology of inhomogeneous space-times without using any of the approximations which are necessary for the hybrid approach. Such a theory would, in addition to providing a better understanding of the link between LQC and LQG, allow one to probe the full behaviour of the universe in high curvature regimes. One could then study the specific case of the loop quantization of space-times that admit arbitrary perturbations around a flat, homogeneous and isotropic background in order to obtain falsifiable predictions which could be compared to observations in our universe.

Appendix A

Parity Symmetries

In nongravitational physics, parity transformations are normally taken to be discrete diffeomorphisms $x_i \to -x_i$ in the physical space which are isometries of the flat 3-metric thereon. In the phase space formulation of general relativity, we do not have a flat metric, or indeed any fixed metric. Therefore these discrete symmetries are no longer meaningful (except in the weak field limit). However, if the dynamical variables have internal indices —such as the triads and connections used in LQG— we can use the fact that the internal space I is a vector space equipped with a flat metric q_{ij} to define parity operations on the internal indices. Associated with any unit internal vector v^i, there is a parity operator Π_v which reflects the internal vectors across the 2-plane orthogonal to v^i. This operation induces a natural action on triads e^a_i, the connections A^i_a and the conjugate momenta $P^a_i =: (1/8\pi G\gamma)\, E^a_i$ (since they are all internal vectors or co-vectors).

The triads e^a_i are proper internal co-vectors. In previous references [86, 105], conventions were such that the spin connection Γ^a_i turned out to be an internal pseudovector. It was then natural to regard the Barbero-Immirzi parameter γ to be a pseudo quantity so that the connection A^i_a has definite parity namely, it transforms as an internal pseudovector. This in turn led to the conclusion that P^a_i is also an internal pseudovector (as one would expect because it is canonically conjugate to A^i_a) [86]. While this is all self-consistent, these conventions lead to two undesirable consequences. First, in the classical theory, it is not possible to reconstruct the triads e^a_i unambiguously starting from the momenta P^a_i. Therefore, one cannot recover the space-time geometry unambiguously starting from the

Hamiltonian theory. Second, the momenta P_i^a are subject to a nonholonomic constraint which obstructs the passage to quantum theory a la LQG. However, if one sets conventions as in Sec. 3.2.1, then $\Gamma_a^i, \gamma, A_a^i$ and P_a^i are all *proper* quantities and the two difficulties disappear [116]. In the main text we have used this strategy.

In diagonal Bianchi models, we can restrict ourselves just to three parity operations Π_i. Under their action, the canonical variables c_i, p_i transform as follows:

$$\Pi_1(c_1, c_2, c_3) = (-c_1, c_2, c_3), \qquad \Pi_1(p_1, p_2, p_3) = (-p_1, p_2, p_3)\,, \tag{A.1}$$

and the action of Π_2, Π_3 is given by cyclic permutations. Thus, c^i and p_i are *proper* internal vectors and co-vectors. Under any of these maps Π_i, the symplectic structure given in Eq. (3.15), the Hamiltonian in Eq. (3.20), and hence also the Hamiltonian vector field, are left invariant. This is just as one would expect because Π_i are simply large gauge transformations of the theory under which the physical metric q_{ab} and the extrinsic curvature K_{ab} do not change. Also, it is clear from the action of Eq. (A.1) that if one knows the dynamical trajectories on the octant $p_i \geq 0$ of the phase space, then dynamical trajectories on any other octant can be obtained just by applying a suitable (combination of) Π_i. Therefore, in the classical theory one can restrict one's attention just to the positive octant.

Let us now turn to the quantum theory. We now have three operators $\hat{\Pi}_i$. Their action on states is given by

$$\hat{\Pi}_1 \Psi(\lambda_1, \lambda_2, \lambda_3) = \Psi(-\lambda_1, \lambda_2, \lambda_3)\,, \tag{A.2}$$

etc. What is the induced action on operators? Since

$$\begin{aligned} \hat{\Pi}_1 \hat{\lambda}_1 \hat{\Pi}_1 \Psi(\lambda_1, \lambda_2, \lambda_3) &= \hat{\Pi}_1 \Big(\lambda_1\, \Psi(-\lambda_1, \lambda_2, \lambda_3)\Big) \\ &= -\lambda_1 \Psi(\lambda_1, \lambda_2, \lambda_3), \end{aligned} \tag{A.3}$$

we have

$$\hat{\Pi}_1 \hat{\lambda}_1 \hat{\Pi}_1 = -\hat{\lambda}_1. \tag{A.4}$$

The Hamiltonian constraint operator, modulo factor ordering which is not important here, is given by Eq. (3.46). To calculate its transformation property under parity maps, in addition to Eq. (A.4), we also need the transformation property of the operators $\sin\bar{\mu}_i c_i$ and $\hat{\varepsilon}$ and operators corresponding to inverse powers of p_1. Due to the symmetries of type A Bianchi models, to know the properties of $\sin\bar{\mu}_i c_i$ under parity transformations, it is sufficient to calculate $\hat{\Pi}_i \sin\bar{\mu}_1 c_1 \hat{\Pi}_i$. We have:

$$\begin{aligned}
\hat{\Pi}_1 \sin\bar{\mu}_1 c_1 \hat{\Pi}_1 \Psi(\lambda_1, \lambda_2, \lambda_3) &= \frac{1}{2i}\,\hat{\Pi}_1 \Big[\Psi(-\lambda_1 + \frac{1}{|\lambda_2\lambda_3|}, \lambda_2, \lambda_3) \\
&\qquad - \Psi(-\lambda_1 - \frac{1}{|\lambda_2\lambda_3|}, \lambda_2, \lambda_3)\Big] \\
&= \frac{1}{2i}\Big[\Psi(\lambda_1 + \frac{1}{|\lambda_2\lambda_3|}, \lambda_2, \lambda_3) - \Psi(\lambda_1 - \frac{1}{|\lambda_2\lambda_3|}, \lambda_2, \lambda_3)\Big] \\
&= -\sin\bar{\mu}_1 c_1 \Psi(\lambda_1, \lambda_2, \lambda_3), \qquad \text{(A.5)}
\end{aligned}$$

whence

$$\hat{\Pi}_1 \sin\bar{\mu}_1 c_1 \hat{\Pi}_1 = -\sin\bar{\mu}_1 c_1. \qquad \text{(A.6)}$$

An identical calculation shows that

$$\begin{aligned}
\hat{\Pi}_2 \sin\bar{\mu}_1 c_1 \hat{\Pi}_2\, \Psi(\lambda_1, \lambda_2, \lambda_3) &= \frac{1}{2i}\,\hat{\Pi}_2 \Big[\Psi(\lambda_1 - \frac{1}{|\lambda_2\lambda_3|}, -\lambda_2, \lambda_3) \\
&\qquad - \Psi(\lambda_1 + \frac{1}{|\lambda_2\lambda_3|}, -\lambda_2, \lambda_3)\Big] \\
&= \frac{1}{2i}\Big[\Psi(\lambda_1 - \frac{1}{|\lambda_2\lambda_3|}, \lambda_2, \lambda_3) - \Psi(\lambda_1 + \frac{1}{|\lambda_2\lambda_3|}, \lambda_2, \lambda_3)\Big] \\
&= \sin\bar{\mu}_1 c_1 \Psi(\lambda_1, \lambda_2, \lambda_3)\,, \qquad \text{(A.7)}
\end{aligned}$$

and similarly for $\hat{\Pi}_3$. Therefore, we have:

$$\hat{\Pi}_2 \sin\bar{\mu}_1 c_1 \hat{\Pi}_2 = \sin\bar{\mu}_1 c_1, \quad \text{and} \quad \hat{\Pi}_3 \sin\bar{\mu}_1 c_1 \hat{\Pi}_3 = \sin\bar{\mu}_1 c_1. \qquad \text{(A.8)}$$

As expected, these transformation properties of $\sin\bar{\mu}_1 c_1$ under $\hat{\Pi}_i$ mirror those of c_1 under the three parity operations Π_i in the classical theory. (Note that, because of the absolute value signs in the expressions (3.39), $\bar{\mu}_i$ do not change under any of the parity maps.) Finally, it is clear from Eq. (3.38) that

$$\hat{\Pi}_i \, \hat{\varepsilon} \, \hat{\Pi}_i = \begin{cases} \hat{\varepsilon} \text{ if } v = 0, \\ -\hat{\varepsilon} \text{ otherwise}, \end{cases} \tag{A.9}$$

and from Eq. (3.55) that

$$\hat{\Pi}_i \, \widehat{|p_1|^{-1/4}} \, \hat{\Pi}_i = \widehat{|p_1|^{-1/4}}. \tag{A.10}$$

[Note incidentally that this need not be the case for factor-ordering choices different from Eq. (3.55).]

We can now collect these results to study the transformation properties of the Hamiltonian constraint. Consider first the regular subspace $\mathcal{H}^{\mathrm{grav}}_{\mathrm{reg}}$ of $\mathcal{H}^{\mathrm{grav}}_{\mathrm{kin}}$ spanned by states which have no support on points with $v = 0$. From Eq. (3.46) it follows that the restriction to $\mathcal{H}^{\mathrm{grav}}_{\mathrm{reg}}$ of the gravitational part of the Hamiltonian constraint is left invariant under $\hat{\Pi}_i$. Since $\hat{p}_T^2$ is manifestly invariant, on the regular subspace we have

$$\hat{\Pi}_i \; \hat{\mathcal{C}}_H \; \hat{\Pi}_i = \hat{\mathcal{C}}_H \tag{A.11}$$

Next, since the gravitational part of the Hamiltonian constraint annihilates the states in the singular subspace (i.e., those with support only on those points at which $v = 0$), we have

$$\hat{\mathcal{C}}_H \Psi = -\hbar^2 \partial_T^2 \Psi = \hat{\Pi}_i \; \hat{\mathcal{C}}_H \; \hat{\Pi}_i \Psi. \tag{A.12}$$

Thus, the Hamiltonian constraint operator is left invariant by all the parity operators, mirroring the behaviour of its classical counterpart.

This invariance implies that, given any state $\Psi \in \mathcal{H}^{\mathrm{grav}}_{\mathrm{kin}}$, the restriction to the positive octant of its image under $\hat{\mathcal{C}}_{\mathrm{grav}}$ determines its image everywhere on $\mathcal{H}^{\mathrm{grav}}_{\mathrm{kin}}$. This property simplifies calculations and was used to arrive at the form of the Hamiltonian constraint given in Eq. (3.69).

Appendix B

The Closed Friedmann-Lemaître-Robertson-Walker Model

The previous treatments of the closed isotropic model [46, 47] obtain the quantum Hamiltonian constraint by expressing the curvature in terms of holonomies. In this appendix we will present an alternate loop quantization of the closed FLRW space-time following the approach used in Chapters 3 and 4 where the connection, rather than the curvature, is expressed by holonomies. This freedom results in a Planck scale ambiguity in the resulting dynamics.

In the first part of this appendix, we derive the LQC Hamiltonian constraint operator for closed FLRW space-times by expressing the connection in terms of holonomies and in the second part we comment on the differences between this quantization procedure and the one followed in [46, 47].

Remark: In the flat FLRW and the Bianchi I models, one obtains the same theory for the two different quantization procedures; on the other hand, the introduction of a connection operator expressed in terms of holonomies is necessary in order to obtain the LQC of open FLRW space-times as well as the Bianchi type II and type IX models. Therefore, this quantization ambiguity is only present in the closed FLRW model.

B.1 The Hamiltonian Constraint Operator

The classical Hamiltonian constraint can be obtained directly from Eq. (4.16) by setting all of the $c_i = c$ and $p_i = p$:

$$\mathcal{C}_H = -\frac{3}{8\pi G\gamma^2}\left(p^2c^2 + \ell_o\varepsilon p^2 c + \frac{\ell_o^2}{4}(1+\gamma^2)p^2\right) + \frac{1}{2}p_T^2 \approx 0, \tag{B.1}$$

and the Poisson bracket for c and p is given by

$$\{c, p\} = \frac{8\pi G\gamma}{3}. \tag{B.2}$$

Working in the momentum representation, p acts by multiplication and the $\hat{c}$ operator is given by [compare with Eq. (4.37)]

$$\hat{c} = \frac{\widehat{\sin\bar{\mu}c}}{\bar{\mu}}, \tag{B.3}$$

where $\bar{\mu} = \sqrt{\Delta\ell_{\rm Pl}^2/|p|}$. Introducing $v = \mathrm{sgn}(p)|p|^{3/2}/2\pi\gamma\sqrt{\Delta}\ell_{\rm Pl}^3$, a symmetric factor ordering gives

$$\begin{aligned}\hat{\mathcal{C}}_H = &-\frac{3\pi\hbar\ell_{\rm Pl}^2}{2}\sqrt{|v|}\sin\bar{\mu}c|v|\sin\bar{\mu}c\sqrt{|v|}\\ &-\frac{3\pi\ell_o\sqrt{\Delta}\hbar\ell_{\rm Pl}^2}{4(2\pi\gamma\sqrt{\Delta})^{1/3}}|v|^{5/6}(\sin\bar{\mu}c\,\hat{\epsilon} + \hat{\epsilon}\sin\bar{\mu}c)|v|^{5/6}\\ &-\frac{3\pi\ell_o^2\Delta(1+\gamma^2)\hbar\ell_{\rm Pl}^2}{8(2\pi\gamma\sqrt{\Delta})^{2/3}}|v|^{4/3} + \frac{1}{2}\hat{p}_T^2,\end{aligned} \tag{B.4}$$

where we have dropped the hats on the v and $\sin\bar{\mu}c$ operators in order to simplify the notation.

It is easy to check that

$$\widehat{e^{-i\bar{\mu}c}}\Psi(v) = \Psi(v+2), \tag{B.5}$$

and it follows that the action of the Hamiltonian constraint operator on a wave function is given by

$$-\hbar^2\partial_T^2\Psi(v;T) = \hat{\Theta}\Psi(v;T), \tag{B.6}$$

where, restricting our attention to the $v \geq 0$ sector,

$$\begin{aligned}\hat{\Theta}\Psi(v;T) = \frac{3\pi\hbar\ell_{\rm Pl}^2}{4}\Bigg[&- \sqrt{v(v+4)}(v+2)\,\Psi(v+4;T) + 2v^2\,\Psi(v;T) \\ &- \sqrt{v|v-4|}(v-2)\,\Psi(v-4;T) \\ &+ \frac{i\ell_o\sqrt{\Delta}}{(2\pi\gamma\sqrt{\Delta})^{1/3}} v^{5/6}\Big[(v+2)^{5/6}\,\Psi(v+2;T) \\ &- \theta_{v-2}|v-2|^{5/6}\,\Psi(v-2;T)\Big] \\ &+ \frac{\ell_o^2\Delta(1+\gamma^2)}{(2\pi\gamma\sqrt{\Delta})^{2/3}} v^{4/3}\,\Psi(v;T)\Bigg]. \end{aligned} \tag{B.7}$$

B.2 Comments on the Different Quantizations

The LQC quantization of the closed FLRW cosmology presented in this appendix differs from the quantization presented in [46, 47] in that it is the connection, rather than the curvature, which is expressed in terms of holonomies.

Following [46, 47], one finds

$$F_{ab}{}^k = \frac{1}{\bar{\mu}^2\ell_o^2}\left(\sin^2\bar{\mu}\left(c - \tfrac{1}{2}\ell_o\right) - \sin^2\left(\tfrac{1}{2}\bar{\mu}\ell_o\right)\right)\mathring{\epsilon}_{ij}{}^k\mathring{\omega}^i_{[a}\mathring{\omega}^j_{b]}; \tag{B.8}$$

using trigonometric identities this can be rewritten as

$$F_{ab}{}^k = \frac{1}{\bar{\mu}^2\ell_o^2}\Big(\sin^2\bar{\mu}c\cos\bar{\mu}\ell_o + \sin\bar{\mu}c\cos\bar{\mu}c\sin\bar{\mu}\ell_o\Big)\mathring{\epsilon}_{ij}{}^k\mathring{\omega}^i_{[a}\mathring{\omega}^j_{b]}. \tag{B.9}$$

On the other hand, following the quantization procedure given in this appendix, one can derive the curvature from Eq. (B.3) which gives a different result:

$$F_{ab}{}^k = \frac{1}{\bar{\mu}^2\ell_o^2}\Big(\sin^2\bar{\mu}c + \bar{\mu}\ell_o\sin\bar{\mu}c\Big)\mathring{\epsilon}_{ij}{}^k\mathring{\omega}^i_{[a}\mathring{\omega}^j_{b]}. \tag{B.10}$$

Clearly, the two expressions only agree in the limit where $\cos\bar{\mu}c$ and $\cos\bar{\mu}\ell_o$ can be approximated by 1 and $\sin\bar{\mu}\ell_o$ can be approximated by $\bar{\mu}\ell_o$.

This quantization ambiguity only becomes important in the Planck regime, but this is precisely where quantum gravity effects are important. Keeping in mind that LQC is only expected to give an approximation to the full dynamics of LQG for symmetry reduced systems, one expects that with more insight from the full theory of LQG and a better understanding of the relation between LQG and LQC, it should be possible to establish which of these two quantizations is the better approximation to the full LQG dynamics (which remain to be determined) of closed homogeneous and isotropic cosmological models.

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Vita

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1. A. Ashtekar and E. Wilson-Ewing, The covariant entropy bound and loop quantum cosmology, Phys. Rev. **D78**, 064047 (2008).

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