TOPICAL REVIEW

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To cite this article: Abhay Ashtekar and Parampreet Singh 2011 *Class. Quantum Grav.* **28** 213001

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Loop quantum cosmology: a status report

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Abstract
Loop quantum cosmology (LQC) is the result of applying principles of loop quantum gravity (LQG) to cosmological settings. The distinguishing feature of LQC is the prominent role played by the *quantum geometry effects* of LQG. In particular, quantum geometry creates a brand new repulsive force which is totally negligible at low spacetime curvature but rises very rapidly in the Planck regime, overwhelming the classical gravitational attraction. In cosmological models, while Einstein's equations hold to an excellent degree of approximation at low curvature, they undergo major modifications in the Planck regime: for matter satisfying the usual energy conditions, any time a curvature invariant grows to the Planck scale, quantum geometry effects dilute it, thereby resolving singularities of general relativity. Quantum geometry corrections become more sophisticated as the models become richer. In particular, in anisotropic models, there are significant changes in the dynamics of shear potentials which tame their singular behavior in striking contrast to older results on anisotropies in bouncing models. Once singularities are resolved, the conceptual paradigm of cosmology changes and one has to revisit many of the standard issues—e.g. the 'horizon problem'—from a new perspective. Such conceptual issues as well as potential observational consequences of the new Planck scale physics are being explored, especially within the inflationary paradigm. These considerations have given rise to a burst of activity in LQC in recent years, with contributions from quantum gravity experts, mathematical physicists and cosmologists. The goal of this review is to provide an overview of the current state of the art in LQC for three sets of audiences: young researchers interested in entering this area; the quantum gravity community in general and cosmologists who wish to apply LQC to probe modifications in the standard paradigm of the early universe. In this review, effort has been made to streamline the material so that

each of these communities can read only the sections they are most interested in, without loss of continuity.

PACS numbers: 04.60.Pp, 04.60.Kz, 04.60.Ds, 98.80.Qc

(Some figures in this article are in colour only in the electronic version)

Contents

Nomenclature

a	scale factor in isotropic models; also the mean scale factor in anisotropic models
a_i	directional scale factors in anisotropic models
A_a^i	gravitational $SU(2)$ connection 1-form on the 3-manifold M, used in LQG
$a, b, \ldots$	spacetime or space indices (in Penrose's abstract index notation)
b	a gravitational phase space variable, conjugate to v, defined in section 2.1
c	symmetry-reduced connection component in isotropic models
c_i	symmetry-reduced connection components in Bianchi models
$\mathcal{C}$	fiducial cell on M, essential in spatially non-compact homogeneous models
C_{grav}	gravitational part of the Hamiltonian constraint
C_H	classical Hamiltonian constraint
$\hat{C}_H$	operator corresponding to C_H
$C_H^{(\text{eff})}$	effective Hamiltonian constraint in LQC, defined in section 5
Δ	ratio of quantum of area to ℓ_{Pl}^2, defined in section 2.5
e_i^a	physical orthonormal triad on M
$\mathring{e}_i^a$	fiducial orthonormal triad on M; $e_i^a = a^{-1}\mathring{e}_i^a$ in isotropic models
E_i^a	physical triad with density weight 1 on M
ϵ	labels super-selected sectors in $\mathcal{H}_{\text{phy}}$, defined in section 2.6
ε	orientation of the triad
ϵ_{jk}^i	structure constants of $SU(2)$
$\mathcal{E}(\nu, \phi; \nu', \phi')$	Green's function obtained from group averaging, defined in section 3.5
F_{ab}^i	curvature of A_a^i
$\hat{F}_{ab}^i$	operator corresponding to F_{ab}^i
$F(x)$	a positive frequency solution of the quantum constraint in sLQC
G	Newton's constant
g_{ab}	spacetime metric
γ	the Barbero–Immirzi parameter of LQG
$\hbar$	Planck's constant divided by 2π
h_ℓ	holonomy of A_a^i along a line segment ℓ
H	Hubble rate
$\hat{H}$	Hamiltonian operator
$\hat{H}_o$	Hamiltonian operator corresponding to the background quantum geometry
$\mathcal{H}_{\text{matt}}$	matter Hamiltonian
$\mathcal{H}_{\text{kin}}$	kinematical Hilbert space
$\mathcal{H}_{\text{kin}}^{\text{grav}}$	gravitational part of the kinematical Hilbert space
$\mathcal{H}_{\text{phy}}$	physical Hilbert space
$i, j, \ldots$	internal $SU(2)$ indices
k	spatial curvature index in isotropic models

k	labels Fourier modes; related to ω as $|k| = \omega/\sqrt{12\pi G}$ in section 2
l_i	proportional to the square root of p_i, defined in section 4.4
L_i	coordinate lengths of $\mathcal{C}$ in the Bianchi models
ℓ_o	cube root of the fiducial volume V_o of the cell $\mathcal{C}$ in $k = 1$ model
$\ell_{\rm Pl}$	Planck's length($\ell_{\rm Pl} = \sqrt{G\hbar/c^3}$)
λ	square root of the quantum of area, defined in section 2.5
Λ	cosmological constant
m	mass parameter
M	spatial manifold
$m_{\rm Pl}$	Planck's mass $m_{\rm Pl} = \sqrt{\hbar c/G}$
μ	dimensionless length of the edge ℓ, along which h_ℓ is computed
$\bar{\mu}$	dimensionless length of the smallest plaquette, defined in section 2.5, also used as an adjective to refer to the 'improved dynamics' in LQC
μ_o	a constant related to the area gap, also used as an adjective to refer to an older dynamics in LQC
N	lapse function
ω	eigenvalue of Θ
$\mathring{\omega}_a^i$	fiducial co-triad, dual to $\mathring{e}_i^a$
$\Omega^{\mu\nu}$	symplectic form on the phase space
p	symmetry-reduced triad component in the isotropic models
$\hat{p}$	operator corresponding to p
p_i	symmetry-reduced triad components in Bianchi models
$\tilde{p}_{(a)}$	canonical conjugate momentum of the scale factor, defined in section 2.1
$p_{(\phi)}$	canonical conjugate momentum of ϕ; Dirac observable for a massless ϕ
$\hat{p}_{(\phi)}$	operator corresponding to the Dirac observable for a massless ϕ
ϕ	a homogeneous scalar field; serves as a relational time variable
ϕ_B	value of the relational time ϕ at which bounce occurs in isotropic models
Φ	an inhomogeneous scalar field
q	determinant of q_{ab}
q_{ab}	physical spatial metric on M
$\mathring{q}_{ab}$	fiducial metric on M
$q_{\pm\bar{k}}, p_{\pm\bar{k}}$	canonically conjugate variables in the Fourier space, defined in section 6.2
R	scalar curvature of the spacetime metric
ρ	energy density
$\hat{\rho}|_\phi$	operator corresponding to the Dirac observable for energy density
$\rho_{\max}$	maximum value of energy density in LQC
σ^2	shear scalar in Bianchi models, defined in section 5.4
$\sigma_{\max}^2$	maximum value of shear scalar
Σ^2	shear parameter in Bianchi models; $\Sigma^2 = \frac{1}{6}\sigma^2 a^6$
t	proper time
τ	harmonic time
$\underline{\Theta}$	quantum constraint operator in the Wheeler–DeWitt theory, defined in section 2.2
Θ	quantum constraint operator in LQC for flat and isotropic models, defined in section 2.5

v	phase space variable corresponding to volume, related to V as $\mathrm{v} = V/(2\pi G)$
$\hat{\mathrm{v}}$	operator corresponding to v
υ	dimensionless volume variable, related to V as $\upsilon = V/(2\pi\gamma\lambda^2\ell_{\mathrm{Pl}})$ used in section 4.4
ν	variable used to define 'volume representation', related to V as $\nu = V/(2\pi\ell_{\mathrm{Pl}}^2)$
$\hat{\nu}$	operator corresponding to ν
V	physical volume of a spatially compact universe, or of the fiducial cell $\mathcal{C}$ in the non-compact case
$\hat{V}$	operator corresponding to V
V_o	volume of the universe, or the cell $\mathcal{C}$, with respect to the fiducial metric $\mathring{q}_{ab}$
$\hat{V}\vert_\phi$	operator corresponding to the Dirac observable for volume at internal time ϕ
$V(\phi)$	scalar field potential
x	proportional to the logarithm of the tangent of $(\lambda\mathrm{b}/2)$, defined in section 3.2
$\mathring{\xi}_i^a$	Killing fields of physical metrics in homogeneous models
y	proportional to the logarithm of b, defined in section 3.1
z	logarithm of volume, defined in section 2.2

1. Introduction

This section is divided into five parts. In the first, we provide a broad overview of how cosmological paradigms have evolved over time and why we need quantum cosmology. In the second, we first discuss potential limitations of restricting quantum gravity considerations to cosmological contexts and explain why quantum cosmology is nonetheless an essential frontier of quantum gravity. In the third, we list some of the most important questions any quantum cosmology theory should address and explain why this challenge has proved to be so non-trivial. In the fourth, we introduce the reader to loop quantum cosmology (LQC) and in the fifth, we provide an outline of how the review is organized to best serve primary interests of three research communities.

1.1. Cosmological paradigms

As recorded history shows, cosmological paradigms have evolved considerably over time as notions of space and time themselves matured. It is illuminating to begin with a broad historical perspective by recalling paradigms that seemed obvious and most natural for centuries only to be superseded by radical shifts.

Treatise on time, the beginning and the end date back at least 25 centuries and it is quite striking that some of the fundamental questions were posed and addressed already in the early literature. Does the flow of time have an objective, universal meaning beyond human perception? Or, is it only a convenient and perhaps merely psychological notion? If it does have an objective meaning, did the physical universe have a finite beginning or has it been evolving eternally? Leading thinkers across cultures meditated on these issues and arrived at definite but strikingly different answers, often rooted in theology. Eastern and Greek traditions generally held that the universe is eternal or cyclic with no beginning or end while the western religions promoted the idea of a finite beginning. A notable variation is St. Augustine who argued in the 4th century CE that time itself started with the world.

Although founding fathers of modern Science, including Galileo and Newton, continued to use theology for motivation and justifications, they nonetheless developed a much more successful paradigm, marked by precision. Before Newton, boundaries between the absolute and the relative and the mathematical and the common were blurry. Through precise axioms stated in the *Pricipia*, Newton isolated time from the psychological *and* the material world, making it objective and absolute. It now ran uniformly from the infinite past to the infinite future, indifferent to matter and forces. This paradigm became the dogma over centuries. The universe came to be identified with matter. Space and time provided an *eternal* background or a stage on which the drama of dynamics unfolds. Philosophers often used this clear distinction to argue that the universe itself *had* to be eternal. For, as Immanuel Kant emphasized, otherwise one could ask 'what was there before?'

As we know, general relativity toppled this paradigm in one fell swoop. Now the gravitational field was encoded in the very geometry of spacetime. Geometry became a dynamical, physical entity and it was now perfectly feasible for the universe to have had a finite beginning—the Big Bang—at which not only matter but *spacetime itself* is born. In this respect, general relativity took us back to St. Augustine's paradigm but in a detailed, specific and mathematically precise form. In books and semi-popular articles, relativists now like to emphasize that the question 'what was there before?' is rendered meaningless because the notion of 'before' requires a pre-existing spacetime geometry. We now have a new paradigm: 'In the beginning there was the Big Bang'.

However, the very fusion of gravity with geometry now gives rise to a new tension. In Newtonian (or Minkowskian) physics, if a given physical field becomes singular at a spacetime point, it cannot be unambiguously evolved to the future but this singularity has no effect on the global arena: since the spacetime geometry is unaffected by matter, it remains intact. Other fields can be evolved indefinitely; trouble is limited to the one field which became ill behaved. However, because gravity is geometry in general relativity, when the gravitational field becomes singular, the continuum tears and the spacetime itself ends. There is no more an arena for other fields to live in. All of physics, as we know it, comes to an abrupt halt. Physical observables associated with both matter and geometry simply diverge, signaling a fundamental flaw in our description of nature.

This problem arises because the reasoning assumes that general relativity—with its representation of spacetime as a smooth continuum—provides an accurate description of nature arbitrarily close to the singularity. But general relativity completely ignores quantum physics and over the last century we have learned that quantum effects become important at high energies. Indeed, they should in fact be *dominant* in parts of the universe where matter densities become enormous. Thus, 'the occurrence of the big-bang and other singularities are predictions of general relativity precisely in a regime where it is inapplicable!' Classical physics of general relativity does come to a halt at the big bang and the big crunch. But this is not an indication of what really happens because the use of general relativity near singularities is an extrapolation which has no physical justification whatsoever. We need a theory that incorporates not only the dynamical nature of geometry but also the ramifications of quantum physics. We need a quantum theory of gravity, a new paradigm[3]. Indeed, cosmological singularities where the spacetime continuum of general relativity simply ends are among the most promising gates to physics beyond Einstein.

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[3] It is sometimes argued that the new paradigm need not involve quantum mechanics or $\hbar$; new classical field equations that do not break down at the big bang should suffice (see e.g. [1]). But well-established physics shows us that quantum theory is essential for the description of matter *much before* one reaches the Planck density, and $\hbar$ features prominently in this description. Stress energy of this quantum matter must couple to gravity. So it is difficult to imagine that a description of spacetime that does not refer to $\hbar$ would be viable in the early universe.

In quantum cosmology, then, one seeks a 'completion' of general relativity, as well as known quantum physics, in the hope that it will provide the next paradigm shift in our overall understanding of the universe. A focus on cosmology serves three purposes. First, the underlying large-scale symmetries of cosmological spacetimes simplify technical issues related to functional analysis. Therefore, it is possible to build mathematically complete and consistent models and systematically explore their physical consequences. Second, the setting is well suited to address the deep conceptual issues in quantum gravity, discussed in subsequent sections, such as the problem of time, extraction of dynamics from a 'frozen' formalism, and the problem of constructing Dirac observables in a background independent theory. These problems become manageable in quantum cosmology and their solutions pave the way to quantum gravity beyond the *S*-matrix theory that background-dependent approaches are wedded to. Finally, the last decade has seen impressive advances in the observational cosmology of the very early universe. As a result, quantum cosmology offers the best avenue available today to confront quantum gravity theories with observations.

1.2. Quantum cosmology: limitations

The first point we just listed to highlight the benefits of focusing quantum gravity considerations to cosmology also brings out a fundamental limitation of this strategy. Symmetry reduction used in the descent from full quantum gravity is severe because it entails ignoring infinitely many degrees of freedom (even in the 'midi-superspaces'). So, a natural question arises: Why should we trust predictions of quantum cosmology? Will results from full quantum gravity resemble anything like what quantum cosmology predicts? There is an early example [2] in which a mini-superspace A was embedded in a larger mini-superspace B and it was argued that quantization of A by itself is inequivalent to the sector of the quantum theory of B that corresponds to A. However, to unravel the relation between the two quantum theories, one should 'integrate out' the extra degrees of freedom in B rather than 'freezing them out'. As an example, let A be the $k = 0$ Friedmann–Lemaître–Robertson–Walker (FLRW) model with a massless scalar field and let B be the Bianchi I model with the same matter source. Then, if one first constructs the quantum theory of the Bianchi I model and *integrates out* the anisotropies in a precise fashion, one does recover the quantum theory of the FLRW model [3]. Thus, a comparison between quantum theories of the larger and the smaller systems has to be carried out with due care. The question is: Will the quantum theory of the smaller system capture the *relevant qualitative features* of the quantum theory of the larger system? We would like to give three arguments which suggest that the answer is likely to be in the affirmative, *provided* quantum cosmology is so constructed that the procedure captures the essential features of the full quantum gravity theory.

First, consider an analogy with electrodynamics. Suppose, hypothetically, that we had full QED but somehow did not have a good description of the hydrogen atom. (Indeed, it is difficult to have a complete control on this bound state problem in the framework of full QED!) Suppose that Dirac came along at this juncture and said: let us first impose spherical symmetry, describe the proton and electron as particles, and then quantize the system. In this framework, all radiative modes of the electromagnetic field would be frozen and we would have quantum mechanics: the Dirac theory of hydrogen atom. One's first reaction would again have been that the simplification involved is so drastic that there is no reason to expect this theory to capture the essential features of the physical problem. Yet we know it does. Quantum cosmology may well be the analog of the hydrogen atom in quantum gravity.

Second, recall the history of singularities in classical general relativity. They were first discovered in highly symmetric models. The general wisdom derived from the detailed analysis

of the school led by Khalatnikov, Lifshitz and others was that these singularities were artifacts of the high symmetry and a generic solution of Einstein's equations with physically reasonable matter would be singularity free. But then singularity theorems of Penrose, Hawking, Geroch and others shattered this paradigm. We learned that lessons derived from symmetry-reduced models were in fact much more general than anyone would have suspected. LQC results on the resolution of the big bang in Gowdy models which have an infinite number of degrees of freedom [4–8], as well as *all* strong curvature singularities in the homogeneous-isotropic context [9], may be hints that the situation would be similar with respect to singularity *resolution* in LQC.

Finally, the Belinskii–Khalatnikov–Lifshitz (BKL) conjecture in classical general relativity says that as one approaches space-like singularities in general relativity, terms in the Einstein equations containing 'spatial derivatives' of basic fields become negligible relative to those containing 'time derivatives' (see, e.g., [10, 11]). Specifically, the dynamics of each spatial point follow the 'Mixmaster' behavior—a sequence of Bianchi I solutions bridged by Bianchi II transitions. By now there is considerable support for this conjecture both from rigorous mathematical and numerical investigations [12–15]. This provides some support for the idea that lessons on the quantum nature of the big-bang (and big-crunch) singularities in Bianchi models may be valid much more generally.

Of course none of these arguments shows conclusively that the qualitative features of LQC will remain intact in the full theory. But they do suggest that one should not *a priori* dismiss quantum cosmology as being too simple. If quantum cosmology is constructed by paying due attention to the key features of a full quantum gravity theory, it is likely to capture qualitative features of dynamics of the appropriate *coarse-grained macroscopic variables*, such as the mean density, the mean anisotropic shears, etc.

1.3. Quantum cosmology: some key questions

Many of the key questions that any approach to quantum gravity should address in the cosmological context were already raised in the seventies by DeWitt, Misner, Wheeler and others. More recent developments in inflationary and cyclic models raise additional issues. In this section, we will present a prototype list. It is far from being complete but provides an approach independent gauge to compare the status of various programs.

- How close to the big bang does a smooth spacetime of general relativity make sense? Inflationary scenarios, for example, are based on a spacetime continuum. Can one show from 'first principles' that this is a safe approximation already at the onset of inflation?
- Is the big-bang singularity naturally resolved by quantum gravity? It is this tantalizing possibility that led to the development of the field of quantum cosmology in the late 1960s. The basic idea can be illustrated using an analogy to the theory of the hydrogen atom. In classical electrodynamics, the ground state energy of this system is unbounded below. Quantum physics intervenes and, thanks to a non-zero Planck's constant, the ground state energy is lifted to a finite value, $-me^4/2\hbar^2 \approx -13.6 \, \text{eV}$. Since it is the Heisenberg uncertainly principle that lies at the heart of this resolution and since the principle is fundamental also to quantum gravity, one is led to ask: Can a similar mechanism resolve the big-bang and big crunch singularities of general relativity?
- Is a new principle/boundary condition at the big-bang or the big-crunch essential? The most well-known example of such a boundary condition is the 'no boundary proposal' of Hartle and Hawking [16]. Or do quantum Einstein equations suffice by themselves even at the classical singularities?

- Do quantum dynamical equations remain well behaved even at these singularities? If so, do they continue to provide a (mathematically) deterministic evolution? The idea that there was a pre-big-bang branch to our universe has been advocated in several approaches (see [17] for a review), most notably by the pre-big-bang scenario in string theory [18], ekpyrotic and cyclic models [19, 20] inspired by the brane world ideas and in theories with high order curvature terms in the action (see eg. [21, 22]). However, these are perturbative treatments which require a smooth continuum in the background. Therefore, their dynamical equations break down at the singularity whence, without an additional input, the pre-big-bang branch is not joined to the current post-big-bang branch by deterministic equations. Can one improve on this situation?
- If there is a deterministic evolution, what is on the 'other side'? Is there just a quantum foam from which the current post-big-bang branch is born, say a 'Planck time after the putative big-bang'? Or, was there another classical universe as in the pre-big-bang and cyclic scenarios, joined to ours by deterministic equations?
- In bouncing scenarios the universe has a contraction phase before the bounce. In general relativity, this immediately gives rise to the problem of growth of anisotropy because the anisotropic shears dominate in Einstein's equations unless one introduces by hand super-stiff matter (see, e.g., [23]). Can this limitation be naturally overcome by quantum modifications of Einstein's equations?

Clearly, to answer such questions we cannot start by assuming that there is a smooth spacetime in the background. But already in the classical theory, it took physicists several decades to truly appreciate the dynamical nature of geometry and to learn to do physics without recourse to a background spacetime. In quantum gravity, this issue becomes even more vexing[4].

For simple systems (including Minkowskian field theories), the Hamiltonian formulation generally serves as a 'royal road' to quantum theory. It was therefore adopted for quantum gravity by Dirac, Bergmann, Wheeler and others. But the absence of a background metric implies that the Hamiltonian dynamics is generated by constraints [29]. In the quantum theory, physical states are solutions to quantum constraints. All of physics, including the dynamical content of the theory, has to be extracted from these solutions. But there is no external time to phrase questions about evolution. Therefore, we are led to ask:

- Can we extract, from the arguments of the wavefunction, one variable which can serve as *emergent time* with respect to which the other arguments 'evolve'? Such an internal or emergent time is not essential to obtain a complete, self-contained theory. But its availability makes the physical meaning of dynamics transparent and one can extract the phenomenological predictions more easily. In a pioneering work, DeWitt proposed that the determinant of the 3-metric can be used as internal time [30]. Consequently, in much of the literature on the Wheeler–DeWitt (WDW) approach to quantum cosmology, the scale factor is assumed to play the role of time, although sometimes only implicitly. However, in closed models, the scale factor fails to be monotonic due to classical recollapse and cannot serve as a global time variable already in the classical theory. Are there better alternatives at least in the simple setting of quantum cosmology?

Finally, there is an important ultraviolet-infrared tension [31]:

- Can one construct a framework that cures the short-distance limitations of classical general relativity near singularities, while maintaining an agreement with it at large scales?

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[4] There is a significant body of literature on this issue; see, e.g., [24–28] and references therein. These difficulties are now also being discussed in the string theory literature in the context of the AdS/CFT conjecture.

By their very construction, perturbative and effective descriptions have no problem with the low energy limit. However, physically their implications cannot be trusted at the Planck scale and mathematically they generally fail to provide a deterministic evolution across the putative singularity. Since non-perturbative approaches often start from deeper ideas, they have the potential to modify classical dynamics in such a way that the big-bang singularity is resolved. But once unleashed, do these new quantum effects naturally 'turn-off' sufficiently fast, away from the Planck regime? The universe has had some *14 billion years* to evolve since the putative big bang and even minutest quantum corrections could accumulate over this huge time period leading to observable departures from dynamics predicted by general relativity. Thus, the challenge to quantum gravity theories is to first create huge quantum effects that are capable of overwhelming the extreme gravitational attraction produced by matter densities of some 10^{94} g cc^{-1} near the big bang, and then switching them off with extreme rapidity as the matter density falls below this Planck scale. This is a huge burden!

In sections 2–6, we will see that all these issues have been satisfactorily addressed in LQC.

1.4. Loop quantum cosmology

Wheeler's geometrodynamics program led to concrete ideas to extract physics from the Dirac–Bergmann approach to canonical quantum gravity already in the seventies [29, 30, 32]. However, mathematically the program still continues to remain rather formal, with little control on the functional analysis that is necessary to adequately deal with the underlying infinite-dimensional spaces, operators and equations. Therefore, the older WDW quantum cosmology did not have guidance from a more complete theory. Rather, since the cosmological symmetry reduction yields a system with only a finite number of degrees of freedom, quantum kinematics was built simply by following the standard Schrödinger theory [33]. Then, as we will see in section 3, the big-bang singularity generically persists in the quantum theory.

The situation is quite different in loop quantum gravity (LQG). In contrast to the WDW theory, a well-established, rigorous kinematical framework *is* available in full LQG [26, 34–36]. If one mimics it in symmetry-reduced models, one is led to a quantum theory which is *inequivalent* to the WDW theory already at the kinematic level. Quantum dynamics built in this new arena agrees with the WDW theory in 'tame' situations but differs dramatically in the Planck regime, leading to new physics. This, in turn, leads to a natural resolution of the big-bang singularity.

These developments occurred in three stages, each of which involved major advances that overcame limitations of the previous one. As a consequence, the viewpoint and the level of technical discussions have evolved quite a bit and some of the statements made in the literature have become outdated. Occasionally, then, there is an apparent tension between statements made at different stages of this evolution. Since this can be confusing to non-experts, we will briefly summarize how the subject evolved. Readers who are not familiar with the LQC literature can skip the rest of this sub-section in the first reading without loss of continuity.

The first and seminal contribution was Bojowald's result [37] that, in the FLRW model, the quantum Hamiltonian constraint of LQC does not break down when the scale factor vanishes and the classical singularity occurs. Since this was a major shift that overcame the impasse of the WDW theory, it naturally led to a flurry of activity and the subject began to develop rapidly (see e.g. [38–44]). This success naturally drew scrutiny. Soon it became clear that these fascinating results came at a cost: it was implicitly assumed that K, the trace of the extrinsic curvature (or the Hubble parameter, $\dot{a}/a$), is periodic, i.e. takes values on a circle

rather than the real line. Since this assumption has no physical basis, at a 2002 workshop at the Schrödinger Institute, doubts arose as to whether the unexpectedly good behavior of the quantum Hamiltonian constraint was an artifact of this assumption.

However, thanks to the key input from Klaus Fredenhagen at the same workshop, it was soon realized [45] that if one mimics the procedure used in full LQG even more closely, the periodicity assumption becomes unnecessary. In the full theory, the requirement of diffeomorphism covariance leads to a *unique* representation of the algebra of fundamental operators [46, 47]. Following the procedure in the full theory, in LQC one finds that K naturally takes values on the real line as one would want physically. But, as mentioned above, the resulting quantum kinematics is *inequivalent* to that of the WDW theory. On this new arena, one can still construct a well-defined quantum Hamiltonian constraint, but now without having to assume the periodicity in K. This new kinematical framework ushered in the second stage of LQC. A number of early papers based on periodicity of K cannot be taken at their face value but results of [45] suggested how they could be reworked in the new kinematical framework. This led to another flurry of activity in which more general models were considered. However, at this stage the framework was analogous to the older WDW theory in one respect: the models did not yet include a physical Hilbert space or well-defined Dirac observables. While there is a general method to introduce the physical inner product on the space of solutions to the quantum constraints [34, 48, 49], it could not be applied directly because often the Hamiltonian constraint failed to be self-adjoint in these models. Consequently, new questions arose. In particular, Brunnemann and Thiemann [50] were led to ask: What is the precise sense in which the physical singularity is resolved?

To address these key physical questions, one needs a physical Hilbert space and a complete family of Dirac observables at least some of which diverge at the singularity in the classical theory. Examples are matter density, anisotropic shears and curvature invariants (all evaluated at an instant of a suitably chosen relational time). The question then is: Do the corresponding operators all remain bounded on the *physical* Hilbert space even in the deep Planck regime? If so, one can say that the singularity is resolved in the quantum theory. In the WDW theory, for example, generically these observables fail to remain bounded whence the singularity is not resolved. What is the situation in LQC?

The third stage of evolution of LQC began with the detailed construction of a mathematical framework to address these issues [51–53]. The physical Hilbert space was constructed using a massless scalar field ϕ as internal time. It was found [52] that the self-adjoint version of the Hamiltonian constraint introduced in the second stage [45]—called the μ_o scheme in the literature—does lead to singularity resolution in the precise sense mentioned above. Since the detailed theory could be constructed, the Hamiltonian constraint could be solved numerically to extract physics in the Planck regime. But this detailed analysis also brought out some glaring limitations of the theory which had remained unnoticed because the physical sector of the theory had not been constructed. (For details see, e.g., appendix 2 of [53], and [54].) In a nutshell, while the singularity was resolved in a well-defined sense, the theory predicted large deviations from general relativity in the low curvature regime: in terms of the key questions raised in section 1.3, it had infrared problems.

Fortunately, the problem could be traced back to the fact that quantization of the Hamiltonian constraint had ignored a conceptual subtlety. Roughly, at a key step in the procedure, the Hamiltonian constraint operator of [45] implicitly used a kinematic 3-metric $\mathring{q}_{ab}$ defined by the co-moving coordinates rather than the physical metric $q_{ab} = a^2 \mathring{q}_{ab}$ (where a is the scale factor). When this is corrected, the new, improved Hamiltonian constraint again *resolves the singularity and, at the same time, is free from all three drawbacks of the μ_o scheme*. This is an excellent example of the deep interplay between physics and mathematics.

The improved procedure is referred to as the '$\bar{\mu}$ scheme' in the literature. The resulting quantum dynamics has been analyzed in detail and has provided a number of insights on the nature of physics in the Planck regime. $\bar{\mu}$ dynamics has been successfully implemented in the case of a non-zero cosmological constant [53, 55–57], the $k = 1$, spatially compact case [58, 59], and to the Bianchi models [3, 60–62]. In the $k = 1$ model, Green and Unruh [31] had laid out more stringent tests that LQC has to meet to ensure that it has good infrared behavior. These were met successfully. Because of these advances, the $\bar{\mu}$ strategy has received considerable attention also from a mathematical physics perspective [63–66]. This work uses a combination of analytic and numerical techniques to enhance rigor to a level that is unprecedented in quantum cosmology.

Over the last 4 years or so LQC has embarked the fourth stage where two directions are being pursued. In the first, the emphasis is on extending the framework to more and more general situations (see, in particular, [3–9, 57, 61, 62, 67]). Already in the spatially homogeneous situations, the transition from μ_o to $\bar{\mu}$ scheme taught us that great care is needed in the construction of the quantum Hamiltonian constraint to ensure that the resulting theory is satisfactory both in the ultraviolet *and* infrared. The analysis of Bianchi models [3, 61, 62] has reinforced the importance of this requirement as a valuable guide. The hope is that these generalizations will guide us in narrowing down choices in the definition of the constraint operator of full LQG. The second important direction is LQC phenomenology. Various LQC effects have been incorporated in the analysis of the observed properties of the cosmic microwave background (CMB) particularly by cosmologists (see, e.g., [68–75]). These investigations explored a wide range of issues, including (i) effects of the quantum-geometry-driven super-inflation just after the big bounce, predicted by LQC; (ii) production of gravitational waves near the big bounce and LQC corrections to the spectrum of tensor modes; and (iii) possible chirality violations. They combine very diverse ideas and are therefore important. However, in terms of heuristics versus precision, there are large variations in the existing literature and the subject is still evolving. As we will see in sections 5 and 6, over the last year or so this frontier has begun to mature. It is likely to become the most active forefront of LQC in the coming years.

1.5. Organization

In section 2, we will introduce the reader to the main issues of quantum cosmology through the $k = 0$ FLRW model [51–53]. We begin with the WDW theory, discuss its limitations and then introduce LQC which is constructed by paying due attention to the Riemannian quantum geometry underlying full LQG. In both cases, we explain how one can use a relational time variable to extract dynamics from the otherwise 'frozen-formalism' of the canonical theory. It turns out that if one uses the relational time variable already in the classical Hamiltonian theory *prior* to quantization, the model becomes exactly soluble also in LQC [76]. Section 3 is devoted to this soluble model. Because the quantization procedure still mimics full LQG and yet the model is solvable analytically, it leads to a direct and more detailed physical understanding of singularity resolution. One can also obtain precise results on similarities and differences between LQC and the WDW theory. We conclude section 3 with a path integral formulation of the model. This discussion clarifies an important conceptual question: How do quantum gravity corrections manage to be dominant near the singularity in spite of the fact that the classical action is large? As we will see, the origin of this phenomenon lies in quantum geometry [77].

Section 4 is devoted to generalizations. We summarize results that have been obtained in a number of models beyond the $k = 0$, FLRW one: the closed $k = 1$ model, models with

cosmological constants with either sign, models with inflationary potentials and the Bianchi models that admit anisotropies [3, 55–58, 61, 62]. In each of these generalizations, new conceptual and mathematical issues arise that initially appear to be major obstacles in carrying out the program followed in the $k = 0$ FLRW case. We explain these issues and provide a succinct summary of how the apparent difficulties are overcome. Although all these models are homogeneous, the increasingly sophisticated mathematical tools that had to be introduced to arrive at a satisfactory LQC provide useful guidance for full LQG.

One of the most interesting outcomes of the detailed analysis of several of the homogeneous models is the power of effective equations [78–80]. They involve only the phase space variables without any reference to Hilbert spaces and operators. Their structure is similar to the constraint and evolution equations in classical general relativity; the quantum corrections manifest themselves only through additional terms that explicitly depend on $\hbar$. As in the classical theory, their solutions provide a smooth spacetime metric and smooth matter fields. Yet, in all cases where the detailed evolution of *quantum* states has been carried out, effective equations have provided excellent approximations to the full quantum evolution of LQC even in the deep Planck regime, provided the states are semi-classical initially in the low curvature regime [53, 55, 56, 58]. Therefore, section 5 is devoted to this effective dynamics and its consequences [9, 54, 81]. It brings out the richness of the Planck scale physics associated with the singularity resolution and also sheds new light on inflationary scenarios [82–84].

Section 6 summarizes the research that goes beyond homogeneity. We begin with a discussion of the one polarization Gowdy models that admit infinitely many degrees of freedom, representing gravitational waves. These models have been analyzed in detail using a 'hybrid' quantization scheme [4–7] in which LQC is used to handle the homogeneous modes that capture the essential non-trivial features of geometry, including the intrinsic time variable, and the familiar Fock theory is used for other modes that represent gravitational waves. Rather surprisingly, this already suffices for singularity resolution; a full LQG treatment of all modes can only improve the situation because of the ultraviolet finiteness that is built into LQG. The current treatment of this model is conceptually important because it brings out the minimal features of quantum geometry that are relevant to the singularity resolution. We then summarize a framework to study general inhomogeneous perturbations in an inflationary paradigm [85]. It encompasses the Planck regime near the bounce where one must use quantum field theory on cosmological *quantum* spacetimes [86]. This analysis has provided a step by step procedure to pass from this more general theory to the familiar quantum field theory on curved, classical spacetimes that is widely used in cosmological phenomenology. Finally, through a few specific examples, we illustrate the ideas that are being pursued to find observational consequences of LQC and, reciprocally, to constrain LQG through observations [70–73, 85, 87, 88].

In section 7, we provide illustrations of the lessons we have learned from LQC for full LQG. These include guidance [3, 53, 58, 59] for narrowing down ambiguities in the choice of the Hamiltonian constraint in LQG and a viewpoint [89] toward entropy bounds that are sometimes evoked as constraints that any satisfactory quantum gravity theory should satisfy [90, 91]. A program to complete the Hamiltonian theory was launched recently [92] based on ideas introduced in [93, 94]. We provide a brief summary because this program was motivated in part by the developments in LQC and the construction of a satisfactory Hamiltonian constraint in LQC is likely to provide further concrete hints to complete this program. Next, we summarize the insights that LQC has provided into spin foams [26, 95] and group field theory [96–98]. In broad terms, these are sum-over-histories formulations of LQG where one integrates over *quantum* geometries rather than smooth metrics. Over the last 3 years, there have been significant advances in the spin foam program [99–101]. LQC provides

an arena to test these ideas in a simple setting. Detailed investigations [102–105] have provided concrete support for the paradigm that underlies these programs and the program has also been applied to cosmology [106–108]. Finally, the consistent histories framework provides a generalization of the 'Copenhagen' quantum mechanics that was developed specifically to face the novel conceptual difficulties of non-perturbative quantum gravity [25, 109]. Quantum cosmology offers a concrete and perhaps the most important context where these ideas can be applied. We conclude section 7 with an illustration of this application [110, 111].

Our conventions are as follows. We set $c = 1$ but generally retain G and $\hbar$ explicitly to bring out the conceptual roles they play in the Planck regime and to make the role of quantum geometry more transparent. We will use Planck units, setting $\ell_{\mathrm{Pl}}^2 = G\hbar$ and $m_{\mathrm{Pl}}^2 = \hbar/G$ (rather than the reduced Planck units often used in cosmology). The spacetime metric has signature $- + + +$. Lowercase indices in the beginning of the alphabet, $a, b, c, \ldots$ refer to spacetime (and usually just spatial) indices while $i, j, k, \ldots$ are 'internal' SU(2) indices. The basis in the su(2) Lie algebra is given by the 2×2 matrices τ^i satisfying $\tau_i \tau_j = \frac{1}{2}\epsilon_{ijk}\tau^k$. We regard the metric (and hence the scale factor) as dimensionless so the indices can be raised and lowered without changing physical dimensions. Most of the plots are taken from original papers and have not been updated.

As mentioned in the abstract, this review is addressed to three sets of readers. Cosmologists who are primarily interested in the basic structure of LQC and its potential role in confronting theory with observations may skip section 2, 3, 5.1 and 6 without loss of continuity. Similarly, mathematically inclined quantum gravity readers can skip sections 5 and 5.4. Young researchers may want to enter quantum gravity through quantum cosmology. They can focus on sections 2, 2.1–2.3, 3.1, 3.2, 4.1, 4.2, 6.1 and 6.2 in the first reading and then return to other sections for a deeper understanding. There are several other complementary reviews in the literature. Details, particularly on the early developments, can be found in [112], a short summary for cosmologists can be found in [113], for general relativists in [114] and for beginning researchers in [115, 116]. Because we have attempted to make this report self-contained, there is some inevitable overlap with some of these previous reviews.

2. k = 0 FLRW cosmology: role of quantum geometry

The goal of this section is to introduce the reader to LQC. Therefore, we will discuss in some detail the simplest cosmological spacetime, the $k = 0$, $\Lambda = 0$ FLRW model with a massless scalar field. We will proceed step by step, starting with the classical Hamiltonian framework and explain the conceptual issues, such as the problem of time in quantum cosmology. We will then carry out the WDW quantization of the model. While it has a good infrared behavior, it fails to resolve the big-bang singularity. We will then turn to LQC. We now have the advantage that, thanks to the uniqueness theorems of [46, 47], we have a well-defined kinematic framework for full LQG. Therefore, we can mimic its construction step by step to arrive at a specific quantum kinematics for the FLRW model. As mentioned in section 1.4, because of quantum geometry that underlies LQG, the LQC kinematics differs from the Schrödinger theory used in the WDW theory. The WDW quantum constraint fails to be well defined in the new arena and we are led to carry out a new quantization of the Hamiltonian constraint that is tailored to the new kinematics. The ensuing quantum dynamics—and its relation to the WDW theory—is discussed in section 3. Since the material covered in this section lies at the foundation of LQC, as it is currently practiced, discussion is deliberately more detailed than it will be in the subsequent sections.

2.1. The Hamiltonian framework

This sub-section is divided into two parts. In the first, we recall the phase space formulation that underlies the WDW theory and in the second we recast it using canonical variables that are used in LQG.

2.1.1. Geometrodynamics. In the canonical approach, the first step toward quantization is a Hamiltonian formulation of the theory. In the $k = 0$ models, the spacetime metric is given by

$$g_{ab}\, \mathrm{d}x^a\, \mathrm{d}x^b \;=\; -\mathrm{d}t^2 + q_{ab}\, \mathrm{d}x^a \mathrm{d}x^b \;\equiv\; -\mathrm{d}t^2 + a^2 \big(\mathrm{d}x_1^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2\big), \qquad (2.1)$$

where q_{ab} is the physical spatial metric and a is the scale factor. Here, the coordinate t is the proper time along the world lines of observers moving orthogonal to the homogeneous slices. In the quantum theory, physical and mathematical considerations lead one to use instead relational time, generally associated with physical fields. In this section, we will use a massless scalar field ϕ as the matter source and it will serve as a physical clock. Since ϕ satisfies the wave equation with respect to g_{ab}, in LQC it is most natural to introduce a *harmonic time coordinate τ* satisfying $\Box\, \tau = 0$. Then, the spacetime metric assumes the form

$$g_{ab}\, \mathrm{d}x^a \mathrm{d}x^b = -a^6\, \mathrm{d}\tau^2 + q_{ab}\, \mathrm{d}x^a\, \mathrm{d}x^b \equiv -a^6\, \mathrm{d}\tau^2 + a^2 \big(\mathrm{d}x_1^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2\big) \qquad (2.2)$$

since the lapse function N_τ, defined by $N_\tau \mathrm{d}\tau = \mathrm{d}t$, is given by a^3. This form will be useful later in the analysis.

In the $k = 0$ FLRW models now under considerations, the spatial topology can either be that of a 3-torus $\mathbb{T}^3$ or $\mathbb{R}^3$. In non-compact homogeneous models, spatial integrals in the expressions of the Lagrangian, Hamiltonian and the symplectic structure all diverge. Therefore, due care is needed in the construction of a Hamiltonian framework [117]. Let us therefore begin with the $\mathbb{T}^3$ topology. Then, the co-moving coordinates define a non-dynamical, fiducial metric $\mathring{q}_{ab}$ via

$$\mathring{q}_{ab}\, \mathrm{d}x^a\, \mathrm{d}x^b = \mathrm{d}x_1^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2 \qquad \text{where} \quad x^a \in [0, \ell_o] \text{ for some fixed } \ell_o. \qquad (2.3)$$

We will set $V_o = \ell_o^3$; this is the volume of $\mathbb{T}^3$ with respect to $\mathring{q}_{ab}$. The physical 3-metric q_{ab} will be written as $q_{ab} = a^2 \mathring{q}_{ab}$. Since we have fixed the fiducial metric with a well-defined gauge choice (unlike in the case with $\mathbb{R}^3$ topology), the scale factor a has a direct physical meaning: $V := a^3 V_o$ is the *physical* volume of $\mathbb{T}^3$.

We can now start with the Hamiltonian framework for general relativity coupled with a massless scalar field and systematically arrive at the following framework for the symmetry-reduced FLRW model. The canonical variables are a and $\tilde{p}_{(a)} = -a\dot{a}$ for geometry and ϕ and $p_{(\phi)} = V\dot{\phi}$ for the scalar field. *Here and in what follows, 'dot' denotes the derivative with respect to proper time t.* The non-vanishing Poisson brackets are given by

$$\{a, \tilde{p}_{(a)}\} \;=\; \frac{4\pi G}{3 V_o}, \qquad \{\phi, p_{(\phi)}\} = 1. \qquad (2.4)$$

Because of symmetries, the (vector or the) diffeomorphism constraint is automatically satisfied and the (scalar or the) Hamiltonian constraint (i.e. the Friedmann equation) is given by

$$C_H = \frac{p_{(\phi)}^2}{2V} - \frac{3}{8\pi G}\, \frac{\tilde{p}_{(a)}^2 V}{a^4} \approx 0\,. \qquad (2.5)$$

Next, let us now consider the $\mathbb{R}^3$ spatial topology. Now, we cannot eliminate the freedom to rescale the Cartesian coordinates x^a and hence that of rescaling the fiducial metric $\mathring{q}_{ab}$. Therefore, the scale factor no longer has a direct physical meaning; only ratios of scale factors do. Also, as mentioned above, volume integrals in the expressions of the action, the

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Hamiltonian and the symplectic structure diverge. A natural viable strategy is to introduce a fiducial cell $\mathcal{C}$ and restrict all integrals to it [117]. Because of the symmetries of the $k = 0$ model, we can let the cell be cubical with respect to every physical metric q_{ab} under consideration on $\mathbb{R}^3$. The cell serves as an infrared regulator which has to be removed to extract physical results by taking the limit $\mathcal{C} \to \mathbb{R}^3$ at the end. We will find that many of the results are insensitive to the choice of the cell; in these cases, the removal of the limit is trivial.

Given $\mathcal{C}$, the phase space is again spanned by the quadruplet $a, \tilde{p}_{(a)}; \phi, p_{(\phi)}$; the fundamental non-vanishing Poisson bracket are again given by (2.4) and the Hamiltonian constraint by (2.5). However, now V_o and V refer to the *volume of the cell* $\mathcal{C}$ with respect to the fiducial metric $\mathring{q}_{ab}$ and the physical metric q_{ab}, respectively. Thus, we now have the possibility of performing two rescalings under which physics should not change:

$$\mathring{q}_{ab} \to \alpha^2 \mathring{q}_{ab} \qquad \mathcal{C} \to \beta^3 \mathcal{C}. \tag{2.6}$$

One may be tempted to just fix the cell by demanding that its fiducial (i.e. coordinate) volume be unit, thereby setting β to 1. But because there is no natural unit of length in classical general relativity, for conceptual clarity (and for manifest dimensional consistency in equations) it is best not to tie the two. Under these recalings, we have the following transformation properties:

$$
\begin{aligned}
a \to \alpha^{-1} a, \qquad &\tilde{p}_{(a)} \to \alpha^{-2} \tilde{p}_{(a)}, \qquad &\phi \to \phi, \\
p_{(\phi)} \to \beta^3 p_{(\phi)}, \qquad &V \to \beta^3 V, \qquad &V_o \to \alpha^3 \beta^3 V_o.
\end{aligned}
\tag{2.7}
$$

Next, let us consider the Poisson brackets and the Hamiltonian constraint. Since the Poisson brackets can be expressed in terms of the symplectic structure on the phase space as $\{f, g\} = \Omega^{\mu\nu} \partial_\mu f \, \partial_\nu g$, we have

$$\Omega^{\mu\nu} \to \beta^{-3} \Omega^{\mu\nu} \quad \text{and} \quad C_H \to \beta^3 C_H. \tag{2.8}$$

Consequently, the Hamiltonian vector field $X_H^\mu = \Omega^{\mu\nu} \partial C_H$ is left invariant under both rescalings. Thus, as one would hope, although elements of the Hamiltonian formulation do make an essential use of the fiducial metric $\mathring{q}_{ab}$ and the cell $\mathcal{C}$, the final equations of motion are insensitive to these choices. By explicitly taking the Poisson brackets, it is easy to verify that we have

$$\frac{\ddot{a}}{a} = -2 \frac{\dot{a}^2}{a^2} = -\frac{16\pi G}{3} \rho \qquad \text{and} \qquad \ddot{\phi} = 0. \tag{2.9}$$

Cosmologists may at first find the introduction of a cell somewhat strange because the classical general relativity makes no reference to it. However, in passage to the quantum theory, we need more than just the classical field equations: we need either a well-defined Hamiltonian theory (for canonical quantization) or a well-defined action (for path integrals) which descends from full general relativity. It is here that a cell enters. In the classical theory, we know from the start that equations of motion do not require a cell; cell-independence of the final physical results is *a priori* guaranteed. But since elements that enter the very construction of the quantum theory require the introduction of a cell $\mathcal{C}$, *a priori* cell dependence can permeate the scalar product and definitions of operators. The theory can be viable only if the final physical results are well defined in the limit $\mathcal{C} \to \mathbb{R}^3$.

2.1.2. Connection dynamics. The basic strategy underlying LQG is to cast general relativity in a form that is close to gauge theories so that (i) we have a unified kinematic arena for describing all four fundamental forces of nature and (ii) we can build quantum gravity by incorporating in it the highly successful non-perturbative techniques based on Wilson loops (i.e. holonomies of connections) [118]. Therefore, as in gauge theories, the configuration variable is a gravitational spin connection A_a^i on a Cauchy surface M and its conjugate

momentum is the electric field E_i^a—a Lie-algebra-valued vector field of density weight 1 on M. A key difference from Yang–Mills theories is that the gauge group SU(2) does not refer to rotations in some abstract internal space, but is in fact the double cover of the rotation group SO(3) in the tangent space of each point of M (where the double cover is taken because LQG has to accommodate fermions). Because of this 'soldering' of the gauge group to spatial geometry, the electric fields now have a direct geometrical meaning: they represent orthonormal triads of density weight 1. Thus, the contravariant physical metric on M is given by $q^{ab} = q^{-1} E_i^a E_j^b \mathring{q}^{ij}$ where q^{-1} is the inverse of the determinant q of the covariant metric q_{ab} and $\mathring{q}^{ij}$ the Cartan–Killing metric on the Lie algebra su(2). To summarize, the canonical pair (q_{ab}, p^{ab}) of geometrodynamics is now replaced by the pair (A_a^i, E_i^a). Because we deal with triads rather than metrics, there is now a new gauge freedom, that of triad rotations. In the Hamiltonian theory, these are generated by a new Gauss constraint.

Let us now focus on the $k = 0$ FLRW model with $\mathbb{R}^3$ spatial topology. Again, a systematic derivation of the Hamiltonian framework requires one to introduce a fiducial cell $\mathcal{C}$, which we again take to be cubical. (As in geometrodynamics, for the $\mathbb{T}^3$ spatial topology this is unnecessary.) As before, let us fix a fiducial metric $\mathring{q}_{ab}$ of signature +,+,+ and let $\mathring{e}_i^a$ and $\mathring{\omega}_a^i$ be the orthonormal frames and co-frames associated with its Cartesian coordinates x^a. The symmetries underlying FLRW spacetimes imply that from each equivalence class of gauge-related homogeneous, isotropic pairs (A_a^i, E_i^a), we can select one such that [45]

$$A_a^i = \tilde{c}\, \mathring{\omega}_a^i \qquad \text{and} \qquad E_i^a = \tilde{p}\, (\mathring{q})^{\frac{1}{2}}\, \mathring{e}_i^a. \qquad (2.10)$$

(In the literature, one often uses the notation δ_i^a for $\mathring{e}_i^a$ and δ_a^i for $\mathring{\omega}_a^i$.) Thus, as one would expect, the gauge invariant information in the canonical pair is again captured in just two functions $(\tilde{c}, \tilde{p})$ of time. They are related to the geometrodynamic variables via

$$\tilde{c} = \gamma \dot{a} \quad \text{and} \quad \tilde{p} = a^2, \qquad (2.11)$$

where $\gamma > 0$ is the so-called Barbero–Immirzi parameter of LQG. Whenever a numerical value is needed, we will set $\gamma \approx 0.2375$, as suggested by the black hole entropy calculations (see, e.g., [35]). It turns out that the equations of connection dynamics in full general relativity are meaningful even when the triad becomes degenerate. Therefore, the phase space of connection dynamics is larger than that of geometrodynamics. In the FLRW models, then, we are also led to enlarge the phase space by allowing physical triads to have both orientations and, in addition, to be possibly degenerate. On this full space, $\tilde{p} \in \mathbb{R}$, and $\tilde{p} > 0$ if E_i^a and $\mathring{e}_i^a$ have the same orientation, $\tilde{p} < 0$ if the orientations are opposite, and $p = 0$ if E_i^a is degenerate.

The LQC phase space is then topologically $\mathbb{R}^4$, naturally coordinatized by the quadruplet $(\tilde{c}, \tilde{p}; \phi, p_{(\phi)})$. The non-zero Poisson brackets are given by

$$\{\tilde{c}, \tilde{p}\} = \frac{8\pi G \gamma}{3 V_o} \qquad \text{and} \qquad \{\phi, p_{(\phi)}\} = 1, \qquad (2.12)$$

where as before V_o is the volume of $\mathcal{C}$ with respect to the fiducial metric $\mathring{q}_{ab}$. As in geometrodynamics, the basic canonical pair depends on the choice of the fiducial metric: under the rescaling (2.6), we have

$$\tilde{c} \to \alpha^{-1} \tilde{c} \qquad \text{and} \qquad \tilde{p} \to \alpha^{-2} \tilde{p}, \qquad (2.13)$$

and the symplectic structure carries a cell dependence. Following [45], it is mathematically convenient to rescale the canonical variables as follows:

$$\text{set} \quad c := V_o^{\frac{1}{3}} \tilde{c}, \quad p := V_o^{\frac{2}{3}} \tilde{p}, \quad \text{so that} \quad \{c, p\} = \frac{8\pi G \gamma}{3}. \qquad (2.14)$$

Then, c, p are insensitive to the choice of $\mathring{q}_{ab}$ and the Poisson bracket between them does not refer to $\mathring{q}_{ab}$ *or to* the cell $\mathcal{C}$. Again because of the underlying symmetries (and our gauge fixing) only the Hamiltonian constraint remains. It is now given by

$$C_H = \frac{p_{(\phi)}^2}{2|p|^{\frac{3}{2}}} - \frac{3}{8\pi G \, \gamma^2} \, |p|^{\frac{1}{2}} \, c^2 \approx 0. \tag{2.15}$$

As before, C_H and the symplectic structure are insensitive to the choice of $\mathring{q}_{ab}$ but they do depend on the choice of the fiducial cell $\mathcal{C}$:

$$\Omega^{\mu\nu} \to \beta^{-3}\Omega^{\mu\nu} \qquad \text{and} \qquad C_H \to \beta^3 C_H. \tag{2.16}$$

Since there is no V_o on the right-hand side of the Poisson bracket (2.14), it may seem surprising that the symplectic structure still carries a cell dependence. But note that $\{c, \ p\} = \Omega^{\mu\nu}\partial_\mu c \partial_\nu p$, and since c, p transform as

$$c \to \beta \, c \quad \text{and} \quad p \to \beta^2 p \tag{2.17}$$

but the Poisson bracket does not change, it follows that $\Omega^{\mu\nu}$ must transform via (2.16).

So the situation with cell dependence is exactly the same as in geometrodynamics: while the classical equations of motion and the physics that follows from them are insensitive to the initial choice of the cell $\mathcal{C}$ used in the construction of the Hamiltonian (or Lagrangian) framework, *a priori* there is no guarantee that the final physical predictions of the quantum theory will also enjoy this property. That they must be well defined in the limit $\mathcal{C} \to \mathbb{R}^3$ is an important requirement on the viability of the quantum theory.

The gravitational variables c, p are directly related to the basic canonical pair $(A_a^i, \ E_i^a)$ in full LQG and will enable us to introduce a quantization procedure in LQC that closely mimics LQG. However, we will find that quantum dynamics of the FLRW model is significantly simplified in terms of a slightly different pair of canonically conjugate variables, (b, v):

$$\mathrm{b} := \frac{c}{|p|^{\frac{1}{2}}}, \quad \mathrm{v} := \frac{|p|^{\frac{3}{2}}}{2\pi G} \, \mathrm{sgn} \, p \qquad \text{so that} \quad \{\mathrm{b}, \ \mathrm{v}\} = 2\gamma, \tag{2.18}$$

where sgn p is the sign of p (1 if the physical triad e_i^a has the same orientation as the fiducial $\mathring{e}_i^a$ and -1 if the orientation is opposite). In terms of this pair, the Hamiltonian constraint becomes

$$C_H = \frac{p_{(\phi)}^2}{4\pi G |\mathrm{v}|} - \frac{3}{4\gamma^2}\mathrm{b}^2|\mathrm{v}| \ \approx 0. \tag{2.19}$$

As with (2.5) and (2.15), canonical transformations generated by this Hamiltonian constraint correspond to time evolution in *proper* time. As mentioned in the beginning of this sub-section, it is often desirable to use other time parameters, say τ. The constraint-generating evolution in τ is $N_\tau C_H$ where $N_\tau = \mathrm{d}t/\mathrm{d}\tau$. Of particular interest is the harmonic time that results if the scalar field is used as an internal clock for which we can set $N = a^3 \propto |\mathrm{v}|$.

We conclude with a remark on triad orientations. Since we do not have any spinor fields in the theory, physics is completely insensitive to the orientation of the triad. Under this orientation reversal, we have $p \to -p$ and $\mathrm{v} \to -\mathrm{v}$. In the Hamiltonian framework, constraints generate gauge transformations in the connected component of the gauge group and these have been gauge-fixed through our representation of A_a^i, E_i^a by c, p. The orientation flip, on the other hand, is a 'large gauge transformation' and has to be handled separately. We will return to this point in section 2.6 in the context of the quantum theory.

2.2. The WDW theory

As remarked in section 1.4, mathematically, full quantum geometrodynamics continues to remain formal even at the kinematical level. Therefore, in quantum cosmology, the strategy was to analyze the symmetry-reduced models in their own right [33, 119, 120] without seeking guidance from the more complete theory. Since the reduced FLRW system has only two configuration space degrees of freedom, field theoretical difficulties are avoided from the start. It appeared natural to follow procedures used in standard quantum mechanics and use the familiar Schrödinger representation of the canonical commutation relations that emerge from the Poisson brackets (2.4). But there is still a small subtlety. Because $a > 0$, its conjugate momentum cannot be a self-adjoint operator on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^+, \mathrm{d}a)$ of square integrable functions $\Psi(a)$: if it did, its exponential would act as a unitary displacement operator $\Psi(a) \to \Psi(a + \lambda)$ forcing the resulting wavefunction to have support on negative values of a for some choice of λ. This difficulty can be easily avoided by working with $z = \ln a^3$ and its conjugate momentum (where we introduced the power of 3 to make comparison with LQC more transparent in section 3). Then, we have

$$z = 3 \ln a, \ \tilde{p}_{(z)} = \frac{a}{3} \tilde{p}_{(a)}, \quad \text{so that} \ \{z, \tilde{p}_{(z)}\} = \frac{4\pi G}{3 V_o} \quad \text{and} \quad C_H = \frac{p_{(\phi)}^2}{2V} - \frac{27 V_o^2}{8\pi G} \frac{\tilde{p}_{(z)}^2}{V} \approx 0.$$

$$(2.20)$$

Now it is straightforward to carry out the Schrödinger quantization. One begins with a kinematic Hilbert space $\mathcal{H}_{\mathrm{kin}}^{\mathrm{wdw}} = L^2(\mathbb{R}^2, \mathrm{d}z \, \mathrm{d}\phi)$ spanned by wavefunctions $\Psi(z, \phi)$. The operators $\hat{z}, \hat{\phi}$ act by multiplication while their conjugate momenta act by ($-\mathrm{i}\hbar$ times) differentiation. The Dirac program for quantization of constrained systems tells us that the physical states are to be constructed from solutions to the quantum constraint equation. Since $1/V$ is a common factor in the expression of C_H, it is simplest to multiply the equation by V before passing to quantum theory. We then have

$$\hat{C}_H \, \underline{\Psi}(z, \phi) = 0 \qquad \text{i.e.} \quad \partial_\phi^2 \underline{\Psi}(z, \phi) = 12\pi G \, \partial_z^2 \underline{\Psi}(z, \phi), \tag{2.21}$$

where underbars will serve as reminders that the symbols refer to the WDW theory. The factor ordering we used in this constraint is in fact independent of the choice of coordinates on the phase space; it is 'covariant' in the following precise sense. The classical constraint is quadratic in momenta, of the form $G^{AB} p_A p_B$ where G^{AB} is the WDW metric on the mini-superspace and the quantum constraint operator is of the form $G^{AB}\nabla_A\nabla_B$ where ∇_A is the covariant derivative associated with G^{AB} [121].

   Note that this procedure is equivalent to using a lapse function $N = a^3$. As explained in the beginning of section 2.1, the resulting constraint generates evolution in harmonic time in the classical theory. Since the scalar field ϕ satisfies the wave equation in spacetime, it is natural to regard ϕ as a relational time variable with respect to which the scale factor a (or its logarithm z) evolves. In more general models, the configuration space is richer and the remaining variables—e.g. anisotropies, other matter fields, density, shears and curvature invariants—can all be regarded as evolving with respect to this relational time variable. However, this is a switch from the traditional procedure adopted in the WDW theory where, since the pioneering work of DeWitt [30], a has been regarded as the internal time variable. But in the closed, $k = 1$ model, since a is double-valued on any dynamical trajectory, it cannot serve as a global time parameter. The scalar field ϕ on the other hand is single valued also in the $k = 1$ case. So, it is better suited to serve as a global clock[5].

---

[5] ϕ shares one drawback with a: it also does not have the physical dimensions of time ($[\phi] = [M/L]^{\frac{1}{2}}$). But in both cases, one can rescale the variable with suitable multiples of fundamental constants to obtain a genuine harmonic time τ.

In the Dirac program, the quantum Hamiltonian constraint (2.21) simply serves to single out *physical* quantum states. But none of them are normalizable on the kinematical Hilbert space $\mathcal{H}_{\text{kin}}^{\text{wdw}}$ because the quantum constraint has the form of a Klein–Gordon equation on the (z, ϕ) space and the wave operator has a continuous spectrum on $\mathcal{H}_{\text{kin}}^{\text{wdw}}$. Therefore, our first task is to introduce a physical inner product on the space of solutions to (2.21). The original Dirac program did not provide a concrete strategy for this task but several are available [122, 123]. The most systematic of them is the 'group averaging method' [34, 48, 49]. Since the quantum constraint (2.21) has the form of a Klein–Gordon equation, as one might expect, the application of this procedure yields, as physical states, solutions to the positive (or negative) frequency square root of the constraint [52],

$$-\mathrm{i}\,\partial_\phi \underline{\Psi}(z, \phi) = \sqrt{\underline{\Theta}}\,\underline{\Psi}(z, \phi) \qquad \text{with} \quad \underline{\Theta} = -12\pi G \partial_z^2, \tag{2.22}$$

where $\sqrt{\underline{\Theta}}$ is the square root of the positive definite operator Θ on $\mathcal{H}_{\text{kin}}^{\text{wdw}}$ defined, as usual, using a Fourier transform. The physical scalar product is given by

$$\langle \underline{\Psi}_1 | \underline{\Psi}_2 \rangle = \int_{\phi=\phi_o} \mathrm{d}z\, \bar{\underline{\Psi}}_1(z, \phi)\underline{\Psi}_2(z, \phi), \tag{2.23}$$

where the constant ϕ_o can be chosen arbitrarily because the integral on the right-hand side is conserved. The physical Hilbert space $\mathcal{H}_{\text{phy}}^{\text{wdw}}$ is the space of normalizable solutions to (2.22) with respect to the inner product (2.23).

Let us summarize. By regarding the scalar field as an internal clock and completing the Dirac program, one can interpret the quantum constraint as providing a Schrödinger evolution (2.22) of the *physical* state $\underline{\Psi}$ with respect to the internal time ϕ. Conceptual difficulties associated with the frozen formalism [29] in the Bergmann–Dirac program are thus neatly bypassed. This is an example of the *deparametrization procedure* which enables one to reinterpret the quantum constraint as an evolution equation with respect to a relational time variable.

Next, we can introduce Dirac observables as self-adjoint operators on $\mathcal{H}_{\text{phy}}^{\text{wdw}}$. Since $\hat{p}_{(\phi)}$ is a constant of motion, it is clearly a Dirac observable. Other useful observables are relational. For example, the observable $\hat{V}|_{\phi_o}$ that defines the physical volume at a fixed instant ϕ_o of internal time ϕ is given by

$$\hat{V}|_{\phi_o}\,\underline{\Psi}(z, \phi) = \mathrm{e}^{\mathrm{i}\sqrt{\underline{\Theta}}\,(\phi-\phi_o)}\,(\mathrm{e}^{\hat{z}}V_o)\,\mathrm{e}^{-\mathrm{i}\sqrt{\underline{\Theta}}\,(\phi-\phi_o)}\,\underline{\Psi}(z, \phi)\,. \tag{2.24}$$

Since classically $V = a^3 V_o = e^z V_o$, conceptually definition (2.24) simply corresponds to evolving the physical state $\underline{\Psi}(z, \phi)$ back to the time $\phi = \phi_o$, operating on it by the volume operator, and evolving the new wavefunction at $\phi = \phi_o$ to all times ϕ. Therefore, the framework enables us to ask and answer physical questions such as: How do the expectation value of (or fluctuations in) the volume or matter density operator evolve with ϕ?

These questions were first analyzed in detail by starting with a unit lapse in the classical theory (so that the evolution is in proper time), quantizing the resulting Hamiltonian constraint operator, and finally re-interpreting the quantum constraint as evolution in the scalar field time [52, 53]. Then, the constraint one obtains has a more complicated factor ordering; although it is analogous to the Klein–Gordon equation in (2.21), $\underline{\Theta}$ is a rather complicated positive definite operator whose positive square root cannot be computed simply by performing a Fourier transform. Therefore, the quantum evolution was carried out using numerics. However, as we have seen, considerable simplification occurs if one uses harmonic time already in the

classical theory. Then, one obtains the simple constraint (2.21) so that the quantum model can be studied analytically[6].

As one would hope, a change of factor ordering only affects the details; qualitative features of results are the same and can be summarized as follows. Consider an expanding classical dynamical trajectory in the a, ϕ space and fix a point a_o, ϕ_o on it at which the matter density (and hence curvature) is very low compared to the Planck scale. At $\phi = \phi_o$, construct a 'Gaussian' physical state $\underline{\Psi}(z, \phi_o)$ which is sharply peaked at this point and evolve it backward and forward in the internal time[7]. Does this wave packet remain sharply peaked at the classical trajectory? The answer is in the affirmative. This implies that the WDW theory constructed here has the correct infrared behavior. This is an interesting and non-trivial feature because even in simple quantum systems, dispersions in physical observables tend to spread rapidly. However, the peakedness also means that in the ultraviolet limit it is as bad as the classical theory: matter density grows unboundedly in the past. In the consistent histories framework, this translates into the statement that the probability for the WDW quantum universes to encounter a singularity is unity, independently of the choice of state [125]. 'In this precise sense, the big-bang singularity is not avoided by the WDW theory'. The analytical calculation leading to this conclusion is summarized in section 3.1.

Remarks.

(1) In the literature, on the WDW theory, the issue of singularity resolution has often been treated rather loosely. For example, it is sometimes argued that the wavefunction vanishes at $a = 0$ [126]. By itself this does not imply singularity resolution because there is no *a priori* guarantee that the physical inner product would be local in a and, more importantly, matter density and curvature may still grow unboundedly at early times. Indeed, even in the classical theory, if one uses harmonic (or conformal) time, the big bang is generally pushed back to the infinite past and so a never vanishes! Also sometimes it is argued that the singularity is resolved because the wavefunction becomes highly non-classical (see, e.g., [126, 127]). Again, this by itself does not mean that the singularity is resolved; one needs to show, e.g., that the expectation values of classical observables which diverge in the classical theory remain finite there. In much of the early literature, the physical inner product on the space of solutions to the constraints was not spelled out whence one could not even begin to systematically analyze the behavior of physical observables.

(2) Notable exceptions are [128, 129] where in the $k = 1$ model with radiation fluid, the physical sector is constructed using a matter variable T as relational time. The Hamiltonian constraint takes the form $(\hat{p}_{(T)} - \hat{H})\psi(a, T) = 0$ where $\hat{H}$ is just the Hamiltonian of the harmonic oscillator. To use the standard results from quantum mechanics of harmonic oscillators, the range of a is extended to the entire real line by assuming that the wavefunction is *antisymmetric* in a. It is then argued that the expectation value of the volume—$\hat{V} = |\hat{a}|^3 V_o$ in our terminology—never vanishes. However, since by definition this quantity could vanish only if the wavefunction has support just at $a = 0$, this property does not imply singularity resolution. As noted above, one should show that operators corresponding to physical observables that diverge in the classical theory are bounded above in the quantum theory. This, to our knowledge, was not shown.

---

[6] Although setting $N = 1$ and using proper time in the classical theory makes quantum theory more complicated, it has the advantage that the strategy is directly meaningful also in the full theory. The choice $N = a^3$, by contrast, does not have a direct analog in the full theory.

[7] Because of the positive frequency requirement, due care is necessary in constructing these 'Gaussian' states. As was pointed out in [124], an approximate analytical argument following equation (3.19) in [52] ignored this subtlety. However, the exact numerical simulation did not; the analytical argument should only be regarded as providing intuition for explaining the general physical mechanism behind the numerical result.

2.3. Bypassing von Neumann's uniqueness

In quantum mechanics of systems with a finite number of degrees of freedom, a theorem due to von Neumann uniquely leads us to the standard Schrödinger representation of the canonical commutation relations. This is precisely the representation used in the WDW theory. The remaining freedom—that of factor ordering the Hamiltonian constraint—is rather limited. Therefore, the fact that the big bang is not naturally resolved in the WDW theory was long taken to be an indication that due to symmetry reduction, quantum cosmology is simply not rich enough to handle the ultraviolet issues near cosmological singularities.

However, like any theorem, the von Neumann uniqueness result is based on some assumptions. Let us examine them to see if they are essential in quantum cosmology. Let us begin with non-relativistic quantum mechanics and, to avoid unnecessary complications associated with domains of unbounded operators, state the theorem using exponentials $U(\sigma)$ and $V(\zeta)$ of the Heisenberg operators $\hat{q}$, $\hat{p}$. The algebra generated by these exponentials is often referred to as the Weyl algebra.

> Let $\mathfrak{W}$ be the algebra generated by one-parameter groups of (abstractly defined) operators $U(\sigma)$, $V(\zeta)$ satisfying relations
>
> $$U(\sigma_1)U(\sigma_2) = U(\sigma_1 + \sigma_2), \qquad V(\zeta_1)V(\zeta_2) = V(\zeta_1 + \zeta_2)$$
> $$U(\sigma)V(\zeta) = e^{i\sigma\zeta} V(\zeta)U(\sigma). \tag{2.25}$$
>
> Then, up to unitary equivalence, there is a unique irreducible representation of $\mathfrak{W}$ on a Hilbert space $\mathcal{H}$ in which $U(\sigma)$, $V(\zeta)$ are unitary *and weakly continuous* in the parameters σ, ζ. Furthermore, this representation is unitarily equivalent to the Schrödinger representation with $U(\sigma) = \exp i\sigma\hat{q}$ and $V(\zeta) = \exp i\zeta\hat{p}$ where $\hat{q}$, $\hat{p}$ satisfy the Heisenberg commutation relations. (For a proof, see, e.g., [130].)

The Weyl relations (2.25) are just the exponentiated Heisenberg commutation relations and the requirements of unitarity and irreducibility are clearly natural. The requirement of weak continuity is also well motivated in quantum mechanics because it is necessary to have well-defined self-adjoint operators $\hat{q}$, $\hat{p}$, representing the position and momentum observables. What about the WDW theory? Since a fundamental assumption of geometrodynamics is that the 3-metric and its momentum be well-defined operators on $\mathcal{H}_{\mathrm{kin}}^{\mathrm{wdw}}$, again, the weak continuity is well motivated. Therefore, in the WDW quantum cosmology, the theorem does indeed lead uniquely to the standard Schrödinger representation discussed in section 2.2.

However, the situation is quite different in the connection dynamics formulation of full general relativity. Here, $\mathfrak{W}$ is replaced by a specific $\star$-algebra $\mathfrak{a}_{\mathrm{hf}}$ (called the holonomy-flux algebra [35, 131, 132]). It is generated by holonomies of the gravitational connections A_a^i along one-dimensional curves and fluxes of the conjugate electric fields E_i^a—which serve as orthonormal triads with density weight 1—across 2-surfaces. Furthermore, even though the system has infinitely many degrees of freedom, thanks to the background independence one demands in LQG, theorems due to Lewandowski, Okolow, Sahlmann and Thiemann [46] again led to a unique representation of $\mathfrak{a}_{\mathrm{hf}}$! A little later, Fleischhack [47] established uniqueness using a $C^\star$ algebra $\mathfrak{W}_F$ generated by holonomies and the exponentials of the electric flux operators, which is analogous to the Weyl algebra $\mathfrak{W}$ of quantum mechanics. As was the case with von Neumann uniqueness, this representation had already been constructed in the 1990s and used to construct the kinematics of LQG [35]. The uniqueness results provided a solid foundation for this framework.

However, there is a major departure from the von Neumann uniqueness. A fundamental property of the LQG representation is that while the holonomy operators $\hat{h}$ are well defined,

there is no local operator $\hat{A}_a^i(x)$ corresponding to the gravitational connection. Since classically the holonomies are (path ordered) exponentials of the connection, uniqueness theorems of [46, 47] imply that the analog of the weak continuity with respect to σ in $U(\sigma)$ *cannot* be met in a background independent dynamical theory of connections. Thus, a key assumption of the von Neumann theorem is violated. As a consequence even after symmetry reduction, we are led to new representations of the commutation relations which replace the Schrödinger theory. LQC is based on this new quantum kinematics.

To summarize, since we have a fully rigorous kinematical framework in LQG, we can mimic it in the symmetry-reduced systems. As we will see in the next sub-section, this procedure forces us to a theory which is inequivalent to the WDW theory already at the kinematical level.

2.4. LQC: kinematics of the gravitational sector

Let us begin by spelling out the 'elementary' functions on the classical phase space which are to have well-defined analogs in quantum theory (without any factor ordering or regularization ambiguities). We will focus on the geometrical variables (c, p) because the treatment of matter variables is the same as in the WDW theory. As in full LQG, the elementary variables are given by holonomies and fluxes. However, because of homogeneity and isotropy, it now suffices to consider holonomies only along edges of the fiducial cell $\mathcal{C}$ and fluxes across faces of $\mathcal{C}$; these functions form a 'complete set' (in the sense that they suffice to separate points in the LQC phase space). Let ℓ be a line segment parallel to the kth edge of $\mathcal{C}$ and let its length w.r.t. *any* homogeneous, isotropic metric q_{ab} on M be μ times the length of the kth edge of $\mathcal{C}$ w.r.t. the *same* q_{ab}. Then, a straightforward calculation shows that the holonomy of the connection $A_a^i = \tilde{c}\,\mathring{\omega}_a^i$ along ℓ is given by

$$h_\ell = \exp\left[\tilde{c}\,\mu V_o^{\frac{1}{3}}\,\tau_k\right] = \cos\frac{\mu c}{2}\mathbb{I} + 2\sin\frac{\mu c}{2}\tau_k, \qquad (2.26)$$

where τ_k is a basis in su(2) introduced in section 1.5 and $\mathbb{I}$ is the identity 2×2 matrix. Hence, it suffices to restrict ourselves only to $\mathcal{N}_\mu(c) := e^{i\mu c/2}$ as elementary functions of the configuration variable c. Next, the flux of the electric field, say E_3^a, is non-zero only across the 1–2 face of $\mathcal{C}$ and is given simply by p. Therefore, following full LQG, we will let the triad-flux variable be simply p. These are the elementary variables which are to have unambiguous quantum analogs, $\hat{\mathcal{N}}_{(\mu)}$ and $\hat{p}$. Their commutation relations are dictated by their Poisson brackets:

$$\{\mathcal{N}_{(\mu)}, p\} = \frac{8\pi i\gamma G}{3}\frac{\mu}{2}\mathcal{N}_{(\mu)} \quad \Rightarrow \quad [\hat{\mathcal{N}}_{(\mu)}, \hat{p}] = -\frac{8\pi\gamma G\hbar}{3}\frac{\mu}{2}\hat{\mathcal{N}}_{(\mu)}. \qquad (2.27)$$

The holonomy flux algebra $\mathfrak{a}$ of the FLRW model is (the free $\star$ algebra) generated by $\hat{\mathcal{N}}_{(\mu)}$, $\hat{p}$ subject to the commutation relations given in (2.27). The idea is to find the representation of $\mathfrak{a}$ which is the analog of the canonical representation of the full holonomy-flux algebra $\mathfrak{a}_{hf}$ [35, 131–133] singled out by the uniqueness theorem of [46]. Now, in LQG, the canonical representation of $\mathfrak{a}_{hf}$ can be constructed using a standard procedure due to Gel'fand, Naimark and Segal [134], and is determined by a specific expectation value (i.e. a positive linear) functional on $\mathfrak{a}_{hf}$. In the FLRW model, one uses the 'same' expectation value functional, now on $\mathfrak{a}$. As one would expect, the resulting quantum theory inherits the salient features of the full LQG kinematics.

We can now summarize this representation of $\mathfrak{a}$. Quantum states are represented by *almost periodic* functions $\Psi(c)$ of the connection c—i.e. countable linear combinations

$\sum_n \alpha_n \exp i\mu_n(c/2)$ of plane waves, where $\alpha_n \in \mathbb{C}$ and $\mu_n \in \mathbb{R}$.[8] The (gravitational) kinematic Hilbert space $\mathcal{H}_{\text{kin}}^{\text{grav}}$ is spanned by these $\Psi(c)$ with a finite norm:

$$||\Psi||^2 = \lim_{D \to \infty} \frac{1}{2D} \int_{-D}^{D} \bar{\Psi}(c)\Psi(c) \, dc = \sum_n |\alpha_n|^2. \tag{2.28}$$

Note that normalizable states are *not* integrals $\int d\mu \, \alpha(\mu) \, e^{i\mu(c/2)}$ but *discrete* sum of plane waves $e^{i\mu(c/2)}$. Consequently, the intersection between $\mathcal{H}_{\text{kin}}^{\text{grav}}$ and the more familiar Hilbert space $L^2(\mathbb{R}, dc)$ of quantum mechanics (or of the WDW theory) consists only of the zero function. Thus, already at the kinematic level, the LQC Hilbert space is *very* different from that used in the WDW theory. An orthonormal basis in $\mathcal{H}_{\text{kin}}^{\text{grav}}$ is given by the almost periodic functions of the connection, $\mathcal{N}_{(\mu)}(c) := e^{i\mu c/2}$. (The $N_{(\mu)}(c)$ are in fact the LQC analogs of the spin network functions in full LQG [135, 136]). They satisfy the relation

$$\langle \mathcal{N}_{(\mu)} | \mathcal{N}_{(\mu')} \rangle \equiv \langle e^{\frac{i\mu c}{2}} | e^{\frac{i\mu' c}{2}} \rangle = \delta_{\mu, \mu'}. \tag{2.29}$$

Again, note that although the basis is of the plane wave type, the right-hand side has a Kronecker delta, rather than the Dirac distribution.

The action of the fundamental operators, however, is the familiar one. The configuration operator acts by multiplication and the momentum by differentiation:

$$\hat{\mathcal{N}}_{(\sigma)}\Psi(c) = \exp \frac{i\sigma c}{2} \Psi(c) \qquad \text{and} \qquad \hat{p}\Psi(c) = -i\frac{8\pi\gamma\ell_{\text{Pl}}^2}{3} \frac{d\Psi}{dc}, \tag{2.30}$$

where, as usual, $\ell_{\text{Pl}}^2 = G\hbar$. The first of these provides a one-parameter family of unitary operators on $\mathcal{H}_{\text{kin}}^{\text{grav}}$ while the second is self-adjoint. Finally, although the action of $\hat{\mathcal{N}}_{(\sigma)}$ is *exactly* the same as in the standard Schrödinger theory, there is a key difference in their properties because the underlying Hilbert spaces are distinct: its matrix elements fail to be continuous in σ at $\sigma = 0$. (For example, the expectation value $\langle \mathcal{N}_{(\mu)}(c) | \hat{\mathcal{N}}_{(\sigma)} | \mathcal{N}_{(\mu)}(c) \rangle$ is zero if $\sigma \neq 0$ but is 1 at $\sigma = 0$.) This is equivalent to saying that $\hat{\mathcal{N}}_{(\sigma)}$ fails to be weakly continuous in σ; this is the assumption of the von Neumann uniqueness theorem that is violated. As a result we cannot introduce a connection operator $\hat{c}$ by taking the derivative of $\hat{\mathcal{N}}_{(\mu)}$ as we do in the Schrödinger (and the WDW) theory. (For further discussion, see [137, 138].)

Since $\hat{p}$ is self-adjoint, it is often more convenient to use the representation in which it is diagonal. Then, quantum states are functions $\Psi(\mu)$ of μ with support only on a *countable* number of points. The scalar product is given by

$$\langle \Psi_1 | \Psi_2 \rangle = \sum_n \bar{\Psi}_1(\mu_n) \, \Psi_2(\mu_n), \tag{2.31}$$

and the action of the basic operators by

$$\hat{\mathcal{N}}_{(\alpha)} \, \Psi(\mu) = \Psi(\mu + \alpha) \qquad \text{and} \qquad \hat{p}\Psi(\mu) = \frac{8\pi\gamma\ell_{\text{Pl}}^2}{6}\mu\Psi(\mu). \tag{2.32}$$

Finally, there is one conceptual subtlety that we need to address. In the WDW theory, $\mu \sim a^2$ is positive while in LQC because of the freedom in the orientation of triads, it takes values on the entire real line. However, as discussed at the end of section 2.1.2, orientation reversal of triads, i.e. map $\mu \to -\mu$, corresponds to large gauge transformations which are not generated by constraints and therefore not eliminated by gauge fixing. Nonetheless, in the absence of fermions, they represent gauge because they do not change physics. In the quantum theory, these large gauge transformations are induced by the 'parity' operator, $\hat{\Pi}$,

---

[8] These functions are called *almost periodic* because the coefficients μ_n are allowed to be arbitrary real numbers, rather than integral multiples of a fixed number. It is interesting to note that this theory of almost periodic functions was developed by the mathematician Harold Bohr, Niels' brother.

with the action $\hat{\Pi}\,\Psi(\mu) = \Psi(-\mu)$. There is a well-established procedure to incorporate large gauge transformations in the Yang–Mills theory: decompose the state space into irreducible representations of this group and discuss each of them separately. In the present case, since $\hat{\Pi}^2 = 1$, we are led to consider wavefunctions which are either symmetric or anti-symmetric under $\hat{\Pi}$. There is no qualitative difference in the physics of these sectors [55]. However, since anti-symmetric wavefunctions vanish at $\mu = 0$ to avoid the wrong impression that the singularity resolution is 'put by hand', in LQC it is customary to work with the symmetric representation. Thus, from now, we will restrict ourselves to states satisfying $\Psi(\mu) = \Psi(-\mu)$.

To summarize, by faithfully mimicking the procedure used in full LQG, we arrive at a kinematical framework for LQG which is inequivalent to the Schrödinger representation underlying WDW theory. We are now led to revisit the issue of singularity resolution in this new quantum arena.

2.5. LQC: gravitational part of the Hamiltonian constraint

In this sub-section, we will construct the quantum Hamiltonian constraint on the gravitational part of the kinematic Hilbert space $\mathcal{H}_{\text{kin}}^{\text{grav}}$. Right at the beginning, we encounter a problem: while expression (2.15) of the classical constraint has a factor c^2, there is no operator $\hat{c}$ on $\mathcal{H}_{\text{kin}}^{\text{grav}}$. To compare the situation with the WDW theory, let us use the representation in which μ (or the scale factor) is diagonal and c is analogous to the momentum p_z. Now, in the WDW theory, $\hat{p}_z$ acts by differentiation: $\hat{p}_z \psi(z) \sim -\mathrm{i}\,\mathrm{d}\Psi/\mathrm{d}z$. But since $\Psi(\mu)$ has support on a *countable* number of points in LQC, we cannot define $\hat{c}\,\Psi(c)$ using $-\mathrm{i}\,\mathrm{d}\Psi/\mathrm{d}\mu$. Thus, because the kinematic arena of LQC is qualitatively different from that of the WDW theory, we need a new strategy.

For this, we return to the key idea that drives LQC: rather than introducing *ab initio* constructions, one continually seeks guidance from full LQG. There, the gravitational part of the Hamiltonian constraint is given by

$$
\begin{aligned}
C_{\text{grav}} &= -\gamma^{-2} \int_{\mathcal{C}} \mathrm{d}^3 x \left[N (\det q)^{-\frac{1}{2}} \epsilon^{ij}{}_k E_i^a E_j^b F_{ab}{}^k \right] \\
&= -\gamma^{-2} V_o^{-\frac{1}{3}} \epsilon^{ij}{}_k \mathring{e}_i^a \mathring{e}_j^b |p|^2 F_{ab}{}^k,
\end{aligned} \tag{2.33}
$$

where in the second step we have evaluated the integral in the FLRW model and, as in the WDW theory, geared the calculation to harmonic time by setting $N = a^3$. The non-trivial term is $F_{ab}{}^k$ ($\sim c^2$ when expanded out using the form (2.10) of the connection). Now, while holonomies are well-defined operators on the kinematic Hilbert space of full LQG, there is no local operator corresponding to the field strength. Therefore, as in gauge theories, the idea is to expresses $F_{ab}{}^k$ in terms of holonomies.

2.5.1. The non-local curvature operator.
Recall first from differential geometry that the a–b component of $F_{ab}{}^k$ can be written in terms of holonomies around a plaquette in the a–b plane:

$$
F_{ab}{}^k = 2 \lim_{Ar_\square \to 0} \mathrm{Tr} \left(\frac{h_{\square_{ij}} - \mathbb{I}}{Ar_\square}\, \tau^k \right) \mathring{\omega}_a^i \mathring{\omega}_b^j, \tag{2.34}
$$

where $Ar_\square$ is the area of the plaquette $\square$. In the FLRW model, because of spatial homogeneity and isotropy, it suffices to compute $F_{ab}{}^k$ at any one point and use square plaquettes that lie in the faces of $\mathcal{C}$ with edges that are parallel to those of $\mathcal{C}$. Then, the holonomy $h_{\square_{ij}}$ around the plaquette $\square_{ij}$ is given by

$$
h_{\square_{ij}} = h_j^{(\bar{\mu})^{-1}} h_i^{(\bar{\mu})^{-1}} h_j^{(\bar{\mu})} h_i^{(\bar{\mu})}, \tag{2.35}
$$

where there is no summation over i, j and $\bar{\mu}$ is the (metric independent) ratio of the length of any edge of the plaquette with the edge length of the cell $\mathcal{C}$. Prior to taking the limit, the expression on the right-hand side of (2.34) can be easily promoted to a quantum operator in LQG or LQC. However, the limit does not exist precisely because the weak continuity with respect to the edge length $\bar{\mu}$ fails. Now, the uniqueness theorems [46, 47] underlying LQG kinematics imply that this absence of weak continuity is a direct consequence of background independence [139]. Furthermore, it is directly responsible for the fact that the eigenvalues of geometric operators—in particular, the area operator—are purely discrete. Therefore, in LQC, the viewpoint is that the non-existence of the limit $Ar_\square \to 0$ in quantum theory is not accidental: quantum geometry simply tells us that we should shrink the plaquette not till the area it encloses goes to zero, but only till it equals the minimum non-zero eigenvalue $\Delta \ell_{\mathrm{Pl}}^2$ of the area operator. That is, the action $\hat{F}_{ab}^k \Psi(\mu)$ is to be determined essentially by the holonomy operator $\hat{h}_{\square_{ij}} \Psi(\mu)$ where the area enclosed by the plaquette $\square$ is $\Delta \ell_{\mathrm{Pl}}^2$ *in the quantum geometry determined by* $\Psi(\mu)$. The resulting $\hat{F}_{ab}{}^k$ would be non-local at the Planck scale and the local curvature used in the classical theory will arise only upon neglecting quantum geometry at the Planck scale, e.g. by coarse-graining of suitable semi-classical states.

To implement this idea it only remains to specify the plaquette, i.e. calculate the value of $\bar{\mu}$ in (2.35) that yields the desired plaquette $\square$.

2.5.2. Determining $\bar{\mu}$.   The strategy is to use a heuristic but well-motivated correspondence between kinematic states in LQG and those in LQC. Fix an eigenstate $\Psi_\alpha(\mu) = \delta_{\mu,\alpha}$ of geometry in the LQC Hilbert space $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$. It represents quantum geometry in which each face of $\mathcal{C}$ has area $|\alpha| (4\pi/3) \gamma \ell_{\mathrm{Pl}}^2$. How would this quantum geometry be represented in full LQG? First, the macroscopic geometry must be spatially homogeneous and, through our initial gauge fixing, we have singled out three axes with respect to which our metrics q_{ab} are diagonal (and to which the cubical cell $\mathcal{C}$ is adapted). 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 figure 1(a)). 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 non-zero label possible, namely $j = 1/2$.

For definiteness, let us consider the 1–2 face S_{12} of the fiducial cell $\mathcal{C}$ which is orthogonal to the x_3 axis (see figure 1(b)). 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 $\Delta \ell_{\mathrm{Pl}}^2$ on this surface, where $\Delta = 4\sqrt{3}\pi\gamma$ [132]. For this LQG state to reproduce the LQC state $\Psi_\alpha(\mu)$ under consideration, S_{12} must be pierced by N edges of the LQG spin network, where N is given by

$$N \Delta \ell_{\mathrm{Pl}}^2 = |p| \equiv \frac{4\pi \gamma \ell_{\mathrm{Pl}}^2}{3} |\alpha|.$$

Thus, we can divide S_{12} into N identical squares each of which is pierced by exactly one edge of the LQG state, as in figure 1(b). Any one of these elementary squares encloses an area $\Delta \ell_{\mathrm{Pl}}^2$ and provides us the required plaquette $\square_{12}$. Recall that the dimensionless length of each edge of the plaquette is $\bar{\mu}$. Therefore, their length with respect to the fiducial metric $\mathring{q}_{ab}$ is $\bar{\mu} V_o^{1/3}$. Since the area of S_{12} with respect to $\mathring{q}_{ab}$ is $V_o^{2/3}$, we have

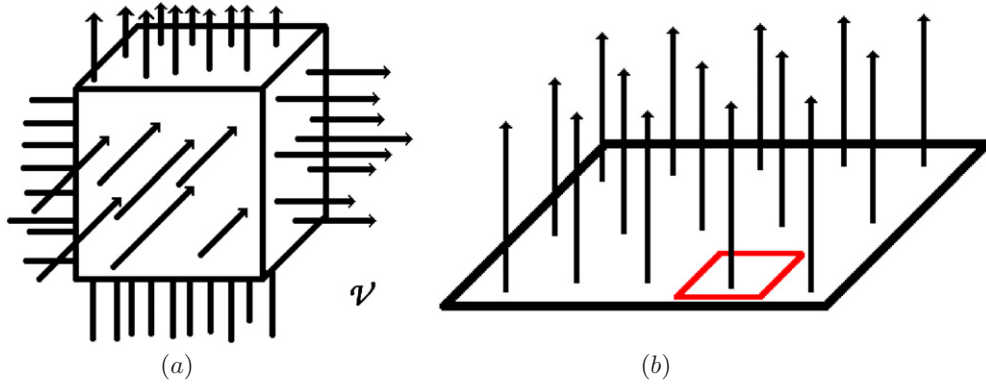$$N (\bar{\mu} V_o^{\frac{1}{3}})^2 = V_o^{\frac{2}{3}}.$$

Figure 1. Depiction of the LQG quantum geometry state corresponding to the LQC state Ψ_α. The LQG spin-network has edges parallel to the edges of the cell $\mathcal{C}$, each carrying a spin label $j = 1/2$. (a) Edges of the spin network traversing through the fiducial cell $\mathcal{C}$. (b) Edges of the spin network traversing the 1–2 face of $\mathcal{C}$ and an elementary plaquette associated with a single flux line. This plaquette encloses the smallest quantum, $\Delta \ell_{\mathrm{Pl}}^2$, of area. The curvature operator $\hat{F}_{12}{}^k$ is defined by the holonomy around such a plaquette.

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

$$\bar{\mu}^2 = \frac{\Delta \ell_{\mathrm{Pl}}^2}{|p|} \equiv \frac{3\sqrt{3}}{|\alpha|}. \tag{2.36}$$

Thus, on a general state $\Psi(\mu)$, the value of $\bar{\mu}$ we should use in (2.35) is given by

$$\bar{\mu} = \left(\frac{3\sqrt{3}}{|\mu|} \right)^{\frac{1}{2}}. \tag{2.37}$$

To summarize, by exploiting the FLRW symmetries and using a simple but well-motivated correspondence between LQG and LQC states, we have determined the unknown parameter $\bar{\mu}$ and hence the required elementary plaquettes enclosing an area $\Delta \ell_{\mathrm{Pl}}^2$ on each of the three faces of the cell $\mathcal{C}$.

2.5.3. The final expression. It is now straightforward to compute the product of holonomies in (2.35) using (2.26) and arrive at the following expression of the field strength operator:

$$\hat{F}_{ab}^k \, \Psi(\mu) = \epsilon_{ij}{}^k \, V_o^{-\frac{2}{3}} \, \mathring{\omega}_a^i \, \mathring{\omega}_b^j \left(\widehat{\frac{\sin^2 \bar{\mu} c}{\bar{\mu}^2}} \right) \Psi(\mu), \tag{2.38}$$

where, for the moment, we have postponed the factor ordering issue. From now on, for notational simplicity, we will generally drop hats over trignometric operators. To evaluate the right-hand side of (2.38) explicitly, we still need to find the action of the operator $\exp[\mathrm{i}\bar{\mu}\,(c/2)]$ on $\mathcal{H}_{\mathrm{kin}}^{\mathrm{total}}$. This is not straightforward because $\bar{\mu}$ is *not* a constant but a function of μ. However, recall that $\mathrm{e}^{\mathrm{i}\mu_o(c/2)}$ is a displacement operator: $\exp[\mathrm{i}\mu_o(c/2)]\,\Psi(\mu) = \Psi(\mu + \mu_o)$. That is, the operator just drags the wavefunction a unit affine parameter distance along the vector field $(\mu_o)\mathrm{d}/\mathrm{d}\mu$. A geometrical argument tells us that the action of $\exp \mathrm{i}\bar{\mu}\,(c/2)$ is completely analogous: it drags the wavefunction a unit affine parameter distance along the vector field $(\bar{\mu})\,\mathrm{d}/\mathrm{d}\mu$. The action on wavefunctions $\Psi(\mu)$ has been spelled out in [53] but is rather complicated. But it was also shown in [53] that the action simplifies greatly if we exploit the fact that the affine parameter is proportional to $|\mu|^{3/2} \sim \mathrm{v}$ (see (2.18)).

The idea then is to make a trivial transition to the volume representation. For later convenience, let us rescale v by setting

$$\nu = \frac{v}{\gamma \hbar} \tag{2.39}$$

and regard states as functions of ν rather than μ. This change to the 'volume representation' is trivial because of the simple form (2.31) of the inner product on $\mathcal{H}_{\text{kin}}^{\text{grav}}$ of LQC. Since the volume representation is widely used in LQC, let us summarize its basic features. The kinematical Hilbert space $\mathcal{H}_{\text{kin}}^{\text{grav}}$ consists of complex-valued functions $\Psi(\nu)$ of $\nu \in \mathbb{R}$ with support only on a countable number of points, and with a finite norm

$$||\Psi||^2 = \sum_n |\Psi(\nu_n)|^2, \tag{2.40}$$

where ν_n runs over the support of Ψ. In this representation, the basic operators are $\hat{V}$, the volume of the fiducial cell $\mathcal{C}$, and its conjugate $\exp i\sigma b$ where σ is a parameter (of dimensions of length) and b is defined in (2.18). The volume operator acts simply by multiplication:

$$\hat{V} \Psi(\nu) = 2\pi \gamma \ell_{\text{Pl}}^2 |\nu| \Psi(\nu), \tag{2.41}$$

while the conjugate operator acts via displacement:

$$[\exp i\sigma b] \, \Psi(\nu) = \Psi(\nu - 2\sigma), \tag{2.42}$$

where σ is a parameter. (b has dimension $[L]^{-1}$ and ν has dimension $[L]$. For details, see [3, 52].) In terms of the original variables c, μ we have $\bar{\mu} c = \lambda b$ where λ is a constant, the square-root of the area gap

$$\lambda^2 = \Delta \ell_{\text{Pl}}^2 = 4\sqrt{3}\pi \gamma \ell_{\text{Pl}}^2, \tag{2.43}$$

whence in the systematic procedure from the μ to the ν representation, the operator $\exp i\bar{\mu} c$ becomes just $\exp i\lambda b$.

Substituting (2.38) in the expression of the gravitational part (2.33) of the Hamiltonian constraint, we obtain

$$\hat{C}_{\text{grav}} \Psi(\nu, \phi) = -24\pi^2 G^2 \gamma^2 \hbar^2 \, |\nu| \frac{\sin \lambda b}{\lambda} |\nu| \frac{\sin \lambda b}{\lambda} \Psi(\nu, \phi), \tag{2.44}$$

where we have chosen a factor ordering analogous to the covariant ordering in the WDW theory.

We will conclude with a discussion of the important features of this procedure and properties of $\hat{C}_{\text{grav}}$.

(1) Since the operator $\hat{F}_{ab}{}^k$ is defined in terms of holonomies and the loop has not been shrunk to zero area, at a fundamental level curvature is non-local in LQC. This non-locality is governed by the area gap and is therefore at a Planck scale. In the classical limit, one recovers the familiar local expression. The size of the loop, i.e. $\bar{\mu}$, was arrived using a semi-heuristic correspondence between LQG and LQC states. This procedure parachutes the area gap from full LQG into LQC; in LQC proper, there is no area gap. It is somewhat analogous to the way Bohr arrived at his model of the hydrogen atom by postulating quantization of angular momentum in a model in which there was no *a priori* basis for this quantization. Recall that although the Bohr model captures some of the essential features of the full, quantum mechanical hydrogen atom, there are also some important differences. In particular, the correct eigenvalues of angular momentum operators are $\sqrt{j(j+1)}\hbar$ rather than $n\hbar$ used by Bohr. Similarly, it is likely that in the final theory, the correct correspondence between full LQG and LQC will require us to use not the 'pure' area gap used here but a more sophisticated coarse-grained version thereof, and

that will change the numerical coefficients in front of $\bar{\mu}$ and the numerical values of various physical quantities such as the maximum density we report in this review. So, specific numbers used in this review should not be taken too literally; they only serve to provide reasonable estimates, help fix parameters in numerical simulations, etc.

(2) The functional dependence of $\bar{\mu}$ on μ on the other hand is robust. Under the rescaling of the fiducial cell, $\mathcal{C} \to \beta^3 \mathcal{C}$, we have $\bar{\mu}c \to \bar{\mu}c$, or equivalently b $\to$ b, whence $\sin \lambda$b does not change and the gravitational part of the constraint simply acquires an overall rescaling as in the classical theory. Had the functional dependence been different, e.g. if we had used $\bar{\mu} = \mu_o$, a constant [45], or $\bar{\mu} \sim |\mu|^{3/2}$ [140], we would have found that b $\to \beta^n$b with $n \neq 0$ whence we would have $\sin \lambda$b $\to \sin \beta^n \lambda$b and the constraint would not have simply rescaled. Consequently, the quantum Hamiltonian constraint would have acquired a non-trivial cell dependence and even in the effective theory (discussed in section 4) physical predictions would have depended on the choice of $\mathcal{C}$. This would have made quantum theory physically inadmissible.

(3) A quick way to arrive at constraint (2.44) is to write the classical constraint in terms of the canonical pair (b, v) (see (2.19)), and then simply replace b by $(\sin \lambda$b$)/\lambda$. While this so-called polymerization method [138, 141] yields the correct final result, it is not directly related to procedures used in LQG because b has no natural analog in LQG. In particular, since it is not a connection component, it would not have been possible to use holonomies to define the curvature operator. For a plausible relation to LQG, one has to start with the canonical pair (A_a^i, E_i^a), i.e. (c, p), mimic the procedure used in LQG as much as possible and then pass to the b representation as was done here. Without this anchor, there is no *a priori* justification for using $\sin \lambda$b$/\lambda$; even if one could argue that b should be replaced by a trigonometric function, there are many other candidates with the same behavior in the $\lambda \to 0$ limit, e.g. $\tan \lambda$b$/\lambda$. However, *a posteriori* it is possible, and indeed often very useful, to use shortcut b $\to (\sin \lambda$ b$)/\lambda$.

2.6. LQC: the full Hamiltonian constraint

We can now add the matter Hamiltonian to obtain the total quantum Hamiltonian constraint using $C_H = C_{\text{grav}} + 16\pi G C_{\text{matt}}$ from the classical phase space formulation [35]. The quantum constraint $\hat{C}_H \Psi(\text{v}, \phi) = 0$ then yields

$$
\begin{aligned}
\partial_\phi^2 \Psi(\nu, \phi) &= 3\pi G \gamma^2 \ \nu \frac{\sin \lambda b}{\lambda} \nu \frac{\sin \lambda b}{\lambda} \Psi(\nu, \phi) \\
&= \frac{3\pi G}{4\lambda^2} \nu [(\nu + 2\lambda)\Psi(\nu + 4\lambda) - 2\nu\Psi(\nu, \phi) + (\nu - 2\lambda)\Psi(\nu - 4\lambda)] \\
&=: -\Theta \Psi(\nu, \phi)
\end{aligned}
\tag{2.45}
$$

where, in the second step, we have used (2.42). Thus, the second order WDW *differential* equation (2.21) is replaced by a second order *difference* equation, where the step size 4λ is dictated by the area gap (which is λ^2). Nonetheless, there is a precise sense in which the WDW equation (2.21)—with its 'covariant' factor ordering—emerges from (2.45) in the limit in which the area gap goes to zero.

Let us begin by setting:

$$
\chi(\nu) := \nu(\Psi(\nu + 2\lambda) - \Psi(\nu - 2\lambda)),
\tag{2.46}
$$

so that (2.45) can be rewritten as

$$
\partial_\phi^2 \Psi(\nu, \phi) = \frac{3\pi G}{4\lambda^2} \nu [\chi(\nu + 2\lambda) - \chi(\nu - 2\lambda)].
\tag{2.47}
$$

To obtain the WDW limit, let us assume $\Psi(\nu)$ is smooth. Then, we have

$$\partial_\phi^2 \Psi(\nu, \phi) = 3\pi G \nu \partial_\nu \chi(\nu) + O\left(\frac{(4\lambda)^n}{n!} \nu \partial_\nu^n \chi\right)$$

$$= 12\pi G \nu \partial_\nu \nu \partial_\nu \Psi + O\left(\frac{(4\lambda)^{m+n}}{m!n!} \nu \partial_\nu^m \nu \partial_\nu^n \Psi(\nu, \phi)\right), \qquad (2.48)$$

where $m, n \geqslant 2$. Thus, if we restrict ourselves to wavefunctions Ψ which are slowly varying in the sense that the 'error terms' under O can be neglected, we obtain the WDW limit of the Hamiltonian constraint (2.45):

$$\partial_\phi^2 \Psi(\nu, \phi) = 12\pi G \; \nu \partial_\nu \; \nu \partial_\nu \Psi(\nu, \phi). \qquad (2.49)$$

This procedure has several noteworthy features. First, in the reduction, in addition to the $\lambda \to 0$ limit, we had to assume that $\Psi(\nu)$ is smooth and slowly varying in ν. Therefore, it cannot be in the LQC Hilbert space $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$. Second, the final form (2.49) of the WDW limit is exactly the same as equation (2.21), including the 'covariant' factor ordering. Third, this approximation is not uniform because the terms which are neglected depend on the state Ψ. However, these assumptions are realized at late times on semi-classical states of interest. In this precise sense, LQC dynamics is well approximated by the WDW theory at late times.

Let us return to LQC. We can now construct the physical Hilbert $\mathcal{H}_{\mathrm{phy}}$ by applying a group averaging procedure [34, 48, 49]. This requires the introduction of an auxiliary Hilbert space $\mathcal{H}_{\mathrm{aux}}$ with respect to which the constraint operator is self-adjoint, which can be achieved simply by a slight modification of the inner product on $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$ to $\langle \Psi_1 | \Psi_2 \rangle = \sum_\nu |\nu|^{-1} \bar\Psi_1(\nu) \Psi_2(\nu)$. (The analogous modification was carried out implicitly in the WDW theory when we considered wavefunctions which are square integrable with respect to the measure $\mathrm{d}z = \mathrm{d}a/a$ in place of $\mathrm{d}a$.) Then, physical states are again those solutions to the 'positive frequency' part of the Hamiltonian constraint,

$$-\mathrm{i}\hbar \partial_\phi \Psi(\nu, \phi) = \sqrt{\Theta} \; \Psi(\nu, \phi), \qquad (2.50)$$

which are symmetric under $\nu \to -\nu$ and have finite norms under the inner product

$$\langle \Psi_1 | \Psi_2 \rangle = \sum_\nu \bar\Psi_1(\nu, \phi_o) \; |\nu|^{-1} \; \Psi_2(\nu, \phi_o). \qquad (2.51)$$

Here, the constant ϕ_o can be chosen arbitrarily because the integral on the right-hand side is conserved. As in the WDW theory, we can again introduce Dirac observables: $\hat{p}_{(\phi)} \equiv \sqrt{\Theta}$, representing the scalar field momentum and, using (2.24), the operator $\hat{V}|_\phi$, representing the volume at internal time ϕ. This completes the specification of the mathematical framework in LQC. One can now explore physical consequences and compare them with those of the WDW theory.

The physics of this quantum dynamics was first studied in detail using computer simulations [53]. Recall that in the classical theory we have two types of solutions: those that start with a big bang and expand forever and their time reversals which begin with zero density in the distant past but collapse into a future, big-crunch singularity (see figure 2(a)). The idea, as in the WDW theory, was to start with a wavefunction which is sharply peaked at a point of an expanding classical solution when the matter density and curvature are very small and evolve the solution backward and forward in the internal time defined by the scalar field ϕ. As in the WDW theory, in the forward evolution, the wavefunction remains sharply peaked on the classical trajectory. Thus, as in the WDW theory, LQC has good infrared behavior. However, in the backward evolution, the expectation value of the volume operator deviates from the classical trajectory once the matter density is in the range 10^{-2}–10^{-3} times the Planck density. Instead of following the classical solution into singularity, the expectation value of volume
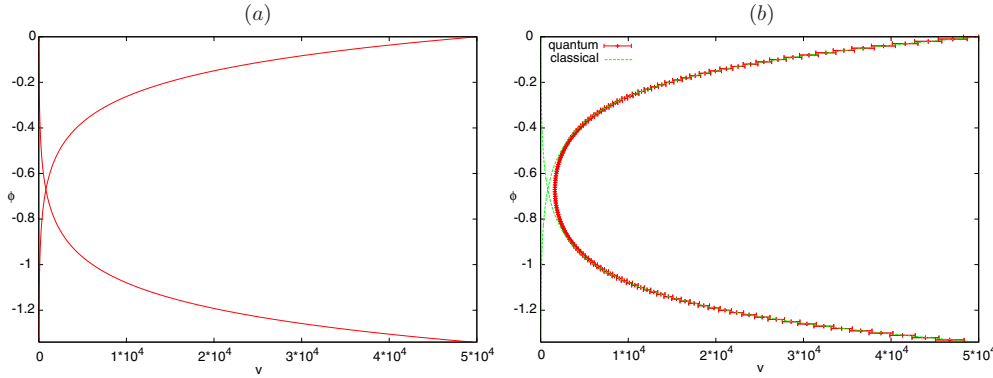
Figure 2. (*a*) Classical solutions in k = 0, $\Lambda = 0$ FRW models with a massless scalar field. Since $p_{(\phi)}$ is a constant of motion, classical trajectories can be plotted in the v–ϕ plane. There are two classes of trajectories. In one, the universe begins with a big bang and expands and in the other it contracts into a big crunch. There is no transition between these two branches. Thus, in a given solution, the universe is either eternally expanding or eternally contracting. (*b*) LQC evolution. Expectation values and dispersion of $|\hat{v}|_\phi$, are compared with the classical trajectory. Initially, the wavefunction is sharply peaked at a point on the classical trajectory at which the density and curvature are very low compared to the Planck scale. In the backward evolution, the quantum evolution follows the classical solution at low densities and curvatures but undergoes a quantum bounce at matter density $\rho \sim 0.41\rho_{Pl}$ and joins on to the classical trajectory that was contracting to the future. Thus, the big-bang singularity is replaced by a quantum bounce.

bounces and soon joins a classical solution which is expanding to the future. Thus, the big bang is replaced by a quantum bounce. Furthermore, the matter density at which the bounce occurs is universal in this model: it is given by $\rho_{max} \approx 0.41\rho_{Pl}$ *independently of the choice of state* (so long as it is *initially* semi-classical in the sense specified above).

The fact that the theory has a good infrared as well as ultraviolet behaviors is *highly* non-trivial. As we saw, the WDW theory fails to have good ultraviolet behavior. Reciprocally, if in place of $\bar{\mu} \sim \mu^{-1/2}$ we had used $\bar{\mu} = \mu_o$, a constant, the big bang would again have been replaced by a quantum bounce but we would not have recovered general relativity in the infrared regime [52]. Indeed, in that theory, there are perfectly good semi-classical states at late times which, even evolved backward, exhibit a quantum bounce at density of water! (See section 7.1.)

A second avenue to explore the Planck scale physics in this model was provided by effective equations, discussed in section 5. While assumptions underlying the original derivation of these equations [78, 79] seem to break down in the Planck regime, as is often the case in physics, these effective equations nonetheless continue to be good approximations to the quantum dynamics of states under consideration for all times. Indeed, the effective equations even provide an analytical expression of the maximum density ρ_{max} whose value is in complete agreement with the exact numerical simulations [53]! A third avenue was introduced subsequently by restricting oneself to a 'superselection sector' (see below) and passing to the representation in which states are functions of b rather than ν [76]. In this representation, one can solve quantum dynamics *analytically* (see section 3). Therefore, one can establish a number of results without the restriction that states be initially semi-classical. One can show that *all* quantum states (in the dense domain of the volume operator) undergo a quantum bounce in the sense that the expectation value of the volume operator has a non-zero lower bound in any state. More importantly, the matter density operator $\hat{\rho}|_\phi$ has a *universal*

upper bound on $\mathcal{H}_{phy}$ and, again, it coincides with ρ_{max} [76]. What is perhaps most interesting is that this upper bound *is induced dynamically*: $\hat{\rho}$ is unbounded on the kinematical Hilbert space. The boundedness implies that in LQC the singularity is resolved in a strong sense: the key observable which diverges at the big bang in the classical theory is tamed and made bounded by quantum dynamics.

Let us summarize. In the simple model under consideration, the scalar field serves as a good clock, providing us with a satisfactory notion of relational time. It enables one to go beyond the 'frozen formalism' in which it is difficult to physically interpret solutions to quantum constraints. Using relational time, one can define Dirac observables, such as the density $\hat{\rho}|_{\phi}$ at the instant ϕ of internal time, and discuss dynamics. We then constructed the physical sector of the WDW theory and found that the singularity is not resolved: if one begins with states which are sharply peaked on a classical solution at late times and evolves them back, one finds that they remain sharply peaked on the classical trajectory all the way to the big bang. In particular, the expectation value of $\hat{\rho}|_{\phi}$ increases unboundedly in this backward evolution. In LQC, by contrast, singularity is resolved in a strong sense: $\hat{\rho}|_{\phi}$ is bounded above on the entire physical Hilbert space! The root of this dramatic difference can be treated directly to quantum geometry that underlies LQG: the bound on the spectrum of $\hat{\rho}|_{\phi}$ is dictated by the 'area gap' and goes to infinity as the area gap goes to zero. Finally, even though the model is so simple, the LQC quantization involves a number of conceptual and mathematical subtleties because one continually mimics the procedures introduced in full LQG.

Remarks.

(1) Note that Θ in (2.45) is a second order difference operator and $(\Theta\Psi)(\nu)$ depends only on values of Ψ at $\nu - 4\lambda$, ν and $\nu + 4\lambda$. Since the physical states also have to be symmetric, $\Psi(\nu, \phi) = \Psi(-\nu, \phi)$, we find that the sub-space $\mathcal{H}_{\epsilon}$ of $\mathcal{H}$, spanned by wavefunctions with support just on the 'lattice' $\nu = \pm\epsilon + 4n\lambda$, is left invariant under dynamics for each $\epsilon \in [0, 4\lambda)$. Furthermore, our complete family of Dirac observables $\hat{p}_{(\phi)}$ and $\hat{V}|_{\phi}$ leaves each $\mathcal{H}_{\epsilon}$ invariant. Thus, the physical Hilbert space $\mathcal{H}_{phy}$ is naturally decomposed into a (continuous) family of separable Hilbert spaces

$$\mathcal{H}_{phy} = \oplus_{\epsilon}\mathcal{H}_{\epsilon}, \qquad \text{with} \quad \epsilon \in [0, 4) \qquad (2.52)$$

and we can analyze each $\mathcal{H}_{\epsilon}$ separately. This property will be used in section 3 to obtain an analytical solution of the problem. Numerical simulations [53] show that as one might expect, qualitative features of physics are insensitive to the choice of ϵ. The key quantitative prediction—value of the maximum density ρ_{max}—is also insensitive.

(2) In this discussion for simplicity, we used the Schrödinger representation for the scalar field. There is also a 'polymer representation' in which the wavefunctions are almost periodic in ϕ. What would have happened if we had used that representation to construct $\mathcal{H}_{kin}^{total}$? It turns out that we would have obtained the same quantum constraint and the same physical Hilbert space $\mathcal{H}_{phy}$.

(3) It is important to note that in LQC, it is the difference equation (2.45) that is fundamental, and it is the continuum limit (2.21) that is physically approximate. This is a reversal of roles from the standard procedure in computational physics. Therefore, some of the statements in [142] addressed to computational physicists can be physically misleading to quantum gravity and cosmology communities. For example, a sentence in the abstract of [142], 'These bounces can be understood as spurious reflections' may be misinterpreted as saying that they are artifacts of bad numerics. This is certainly not the case because numerics in [53] were performed with all due care and furthermore the results are in complete agreement with the analytical solutions found later [76]. Rather, the intent

of that phrase was to say: 'had the physical problem been to solve a wave equation in the *continuum* and had one used non-uniform grids, one would also have found bounces which, from the perspective of continuum physics of this hypothetical problem, would be interpreted as spurious reflections in finite difference discretizations'. This is an illuminating point for computational physicists but is not physically relevant in LQC where the basic equation is a difference equation.

3. Exactly soluble LQC

In this section, we continue with the $k = 0$, $\Lambda = 0$ FLRW model. This model can be solved *exactly* if one uses the scalar field as an internal clock already in the classical theory, prior to quantization, and works in a suitable representation [76]. This analytical control on the quantum theory allows us to prove further results such as the generic character of the bounce, obtain an analytical expression of the upper bound of the energy density operator and carry out a detailed comparison between the WDW theory and soluble LQC (sLQC). Furthermore, questions regarding the behavior of fluctuations and preservation of semi-classicality across the bounce can be answered in detail.

In section 3.1, we recast the WDW quantum constraint in terms of variables that facilitate the comparison with sLQC. In section 3.2, we carry out the loop quantization of this model following [76]. Interestingly, the form of the quantum constraint and the inner product are strikingly similar in the WDW theory and sLQC, yet they lead to very different physical predictions. The reason is that the physical observables directly relevant to cosmology are represented by very different operators in the two cases. Physical predictions of both theories are discussed in section 3.3. In section 3.4, we spell out the precise relation between sLQC and WDW theory and show that the latter does not follow as a limit of the former. There is some apparent tension between the singularity resolution in LQC and the intuition derived from path integrals on the regime in which quantum effects become important. This issue and its resolution are discussed in section 3.5.

Since cosmologists would not have already read section 2, we have attempted to make this section self-contained. For others we have included remarks connecting this discussion with that of section 2.

3.1. The WDW theory

Let us begin by briefly recalling the Hamiltonian framework and fixing notation. (For clarifications and details, see section 2.1.1.)

If the spatial topology is $\mathbb{R}^3$, all spatial integrals diverge in the Hamiltonian (as well as Lagrangian) framework. A standard attitude in much of the older literature was just to ignore this infinity. But then typically quantities on the two sides of equations have different physical dimensions and there are hidden inconsistencies. In a systematic treatment, one has to first introduce an elementary cell $\mathcal{C}$, restrict all integrals to it, construct the theory and in the final step remove this infrared regulator by taking the limit $\mathcal{C} \to \mathbb{R}^3$.

Let us recall that in the canonical framework the WDW phase space is coordinatized by $(a, \tilde{p}_a; \phi, p_{(\phi)})$. The scale factor relates the physical 3-metric q_{ab} to the fiducial one $\mathring{q}_{ab}$, associated with the co-moving coordinates via $q_{ab} = a^2 \mathring{q}_{ab}$. It turns out that in LQC, it is more convenient to work with orthonormal triads rather than 3-metrics and with the physical volume V of $\mathcal{C}$ rather than the scale factor. To facilitate the comparison between the two quantum theories, we will begin by writing the WDW theory in canonical variables which are adapted to LQC. Thus, the gravitational configuration variable will be $v = \varepsilon(V/2\pi G)$

where $\varepsilon = \pm 1$ depending on the orientation of the physical triad, and V is related to the scale factor a via $V = a^3 V_o$, where V_o is the volume of $\mathcal{C}$ in co-moving coordinates. The conjugate momentum $b = \gamma \dot{a}/a$ is the Hubble parameter, except for a multiplicative constant γ, the Barbero–Immirzi parameter of LQG (whose value $\gamma \approx 0.2375$ is fixed by the black hole entropy calculation).

Thus, the full phase space is topologically $\mathbb{R}^4$, coordinatized by $(v, b; \phi, p_{(\phi)})$, and the fundamental Poisson brackets are

$$\{b, v\} = 2\gamma \qquad \text{and} \qquad \{\phi, p_{(\phi)}\} = 1. \tag{3.1}$$

Since we wish to use the scalar field ϕ as emergent time, it is natural to consider evolution in a harmonic time coordinate τ satisfying $\Box \tau = 0$. The associated lapse is then $N_\tau = a^3$ and the Hamiltonian constraint is given by

$$p_{(\phi)}^2 - 3\pi G \, v^2 b^2 = 0. \tag{3.2}$$

Let us use quantum states which are diagonal in b. Then, the quantum constraint becomes

$$\partial_\phi^2 \, \underline{\chi}(b, \phi) = -12\pi G (b \, \partial_b)^2 \, \underline{\chi}(b, \phi), \tag{3.3}$$

where on the right-hand side we have used a 'covariant' factor ordering (as in section 2.2) and the underbars are again served to emphasize that discussing the WDW theory. The change of orientation of triads corresponds to a large gauge transformation under which the physics of the model is unchanged. This turns out to imply that the wavefunctions $\underline{\chi}(b, \phi)$ must satisfy $\underline{\chi}(b, \phi) = -\underline{\chi}(-b, \phi)$ [76]. Therefore, we can incorporate the invariance under large gauge transformations *simply by restricting ourselves to the positive* b-*half-line.*

Constraint (3.3) can be written in a simpler form by introducing

$$y := \frac{1}{(12\pi G)^{1/2}} \ln \frac{b}{b_o}, \tag{3.4}$$

where b_o is an arbitrarily chosen but fixed constant. Since $b \in (0, \infty)$, y is well defined and takes values on the *full real line.* Then, the WDW constraint takes the form of a two-dimensional Klein–Gordon equation as in section 2.2:

$$\partial_\phi^2 \underline{\chi}(y, \phi) = \underline{\Theta} \, \underline{\chi}(y, \phi), \qquad \text{where} \quad \underline{\Theta} := \partial_y^2. \tag{3.5}$$

The idea again is to interpret this equation as providing us with the evolution of $\underline{\chi}(y, \phi)$ in 'relational time' ϕ. Using Fourier transform, one can naturally decompose solutions to (3.5) positive and negative frequency sectors. As explained in section 2, a general 'group averaging' procedure [34, 48, 49] leads us to the physical Hilbert space: $\mathcal{H}_{\text{phy}}^{\text{wdw}}$ consists of positive frequency solutions to (3.5), i.e. solutions satisfying the positive square root - $i\partial_\phi \underline{\chi}(y, \phi) = \sqrt{\underline{\Theta}} \, \underline{\chi}(y, \phi)$ of (3.5), where $\sqrt{\underline{\Theta}} = \sqrt{-\partial_y^2}$ can be easily defined by making a Fourier transform. Since we are working with positive frequency solutions, the physical inner product is given by the standard Klein–Gordon current. In the momentum space, it can be written as

$$(\underline{\chi}_1, \underline{\chi}_2)_{\text{phy}} = 2 \int_{-\infty}^{\infty} dk |k| \bar{\tilde{\underline{\chi}}}_1(k) \tilde{\underline{\chi}}_2(k), \tag{3.6}$$

where $\tilde{\underline{\chi}}$ is the Fourier transform of $\underline{\chi}$ and k is related to the eigenvalues ω of $\underline{\Theta}$ as $\omega = \sqrt{12\pi G}|k|$. This expression is just what one would expect from the two-dimensional Klein–Gordon theory. Finally, general initial datum for the physical state at time $\phi = \phi_o$ is of the form $\underline{\chi}(y, \phi_o) = (1/\sqrt{2\pi}) \int_{-\infty}^{\infty} dk \, e^{-iky} \tilde{\underline{\chi}}(k)$, and under time evolution one obtains

$$\underline{\chi}(y, \phi) = \frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{0} dk \, e^{-ik(\phi+y)} \, e^{ik\phi_o} \tilde{\underline{\chi}}(k) + \int_{0}^{\infty} dk \, e^{ik(\phi-y)} \, e^{-ik\phi_o} \tilde{\underline{\chi}}(k) \right), \tag{3.7}$$

where the first term is a left moving solution while the second is a right moving solution. Thus, $\mathcal{H}_{\text{phy}}^{\text{wdw}}$ can itself be decomposed into two orthogonal subspaces consisting of right and left moving modes.

As in section 2.2, one can introduce a family of Dirac observables. Since $\hat{p}_{(\phi)}$ is a constant of motion, it is trivially a Dirac observable. On $\mathcal{H}_{\text{phy}}^{\text{wdw}}$ its action is given by

$$\hat{p}_{(\phi)} \, \underline{\chi}(y, \phi) = \hbar \sqrt{\underline{\Theta}} \underline{\chi}(y, \phi). \tag{3.8}$$

The second Dirac observable is $\hat{V}|_{\phi_o}$, the volume of the cell $\mathcal{C}$ at time ϕ_o. To define it, we must first introduce the volume operator $\hat{V} = 2\pi G |\widehat{\text{v}}| = 2\pi \gamma \ell_{\text{Pl}}^2 |\widehat{\nu}|$ where, to facilitate comparison with section 2, we have set $\hat{\nu} := \text{v}/\hbar$. In the b representation, $\hat{\nu}$ is simply the self-adjoint-part of $(-2i\partial_b)$, which, in the y representation, becomes

$$\hat{\nu} = -\frac{2}{\sqrt{12\pi G}b_o}(P_R(e^{\sqrt{12\pi G}y}i\,\partial_y)P_R + P_L(e^{\sqrt{12\pi G}y}i\,\partial_y)P_L), \tag{3.9}$$

where P_R and P_L project on the right and left moving, mutually orthogonal subspaces. The second Dirac observable, the volume at internal time ϕ_o, is obtained by 'freezing' the given state $\underline{\chi}(y, \phi)$ at time ϕ_o, operating it by the volume operator, and then evolving the result to obtain a positive frequency solution to (3.5):

$$\hat{V}|_{\phi_o} \, \underline{\chi}(y, \phi) = e^{i\sqrt{\underline{\Theta}}(\phi-\phi_o)}\big(2\pi \gamma \ell_{\text{Pl}}^2 |\hat{\nu}|\big)\underline{\chi}(y, \phi_o), \tag{3.10}$$

Both the Dirac observables are self-adjoint with respect to (3.6) as they must be and, furthermore, *preserve the left and right moving sectors* of $\mathcal{H}_{\text{phy}}^{\text{wdw}}$. Therefore, if one describes physics using this complete set of Dirac observables, it suffices to work with just one sector at a time. This fact is conceptually important since, as we will see that the right sector corresponds to contracting universes and left to expanding [76].

3.2. Loop quantization

We can now turn to LQC in the b representation. The underlying phase space is the same but passage to quantum theory is different because, by following the procedure used in full LQG [46, 47] in this cosmological context, we are led to a theory which is distinct from the WDW theory already at the kinematical level. As a consequence, as we saw in section 2, support of the LQC wavefunctions $\Psi(\nu, \phi)$ in the volume representation can be restricted to regular 'lattices', $\nu = \pm\epsilon + 4n\lambda$ with $\epsilon \in [0, 4\lambda)$, and each ϵ-sector is left invariant by the two Dirac observables *and* evolution. The step size on these lattices is dictated by λ where $\lambda^2 = 4\sqrt{3}\pi \gamma \ell_{\text{Pl}}^2$ is the 'area gap', i.e. the lowest eigenvalue of the area operator in LQG. Thus, while evolution in the WDW theory is governed by a *differential* equation, that in LQC is by a *difference* equation. The advantage of the b representation is that the LQC evolution is again governed by a differential equation and can be compared more directly with that in the WDW theory.

To pass to the b representation, it is simplest to work with the $\epsilon = 0$ lattice [76]. (While some technical details depend on the choice of ϵ, physics is essentially independent.) Then, since $\Psi(\nu, \phi)$ have support on $\nu = 4n\lambda$, their Fourier transform have support on a *circle*: while we have $b \in (-\infty, \infty)$ in the WDW theory, in LQC we have $b \in (0, \pi/\lambda)$. But the quantum Hamiltonian constraint is a differential equation as in the WDW theory:

$$\partial_\phi^2 \chi(b, \phi) = 12\pi G \left(\frac{\sin \lambda b}{\lambda}\partial_b\right)^2 \chi(b, \phi). \tag{3.11}$$

As in the case of the WDW theory, we can make a change of coordinates to rewrite this constraint as a Klein–Gordon equation: in terms of the variable x,

$$x = \frac{1}{\sqrt{12\pi G}} \ln\left(\tan\frac{\lambda b}{2}\right) \tag{3.12}$$

the quantum constraint becomes

$$\partial_\phi^2 \chi(x,\phi) = -\Theta \chi(x,\phi), \qquad \text{where} \qquad \Theta := -\partial_x^2. \tag{3.13}$$

Since $b \in (0, \pi/\lambda)$, it follows that $x \in (-\infty, \infty)$. The requirement that physics should be invariant under the change of orientation of the triad now implies $\chi(x,\phi) = -\chi(-x,\phi)$. This is in striking contrast with the situation in the WDW theory, where this requirement was already used in the very definition of y and left no restriction on $\underline{\chi}(y,\phi)$. It is easy to verify that this restriction implies that the LQC wavefunctions $\chi(x,\phi)$ *must have support on both the right and the left moving sectors*.

Thus, the physical Hilbert space $\mathcal{H}_{\text{phy}}$ now consists of all anti-symmetric, positive frequency solutions to (3.13), i.e. $\chi(x,\phi)$ satisfying $\chi(x,\phi) = -\chi(-x,\phi)$ and $-i\partial_\phi \chi(x,\phi) = \sqrt{\Theta}\chi(x,\phi)$, with a finite norm in the inner product (3.6). The symmetry requirement implies that every solution $\chi(x,\phi)$ can be written as

$$\chi(x,\phi) = \tfrac{1}{\sqrt{2}}(F(x_+) - F(x_-)), \tag{3.14}$$

where F satisfies (3.13) and $x_\pm = \phi \pm x$; the right and left moving parts of $\chi(x,\phi)$ determines its right moving part and vice versa. Therefore, the inner product can then be expressed in terms of the right moving (or left moving) part alone:

$$(\chi_1, \chi_2)_{\text{phys}} = -2i \int_{-\infty}^{\infty} dx \, \bar{F}_1(x_+) \partial_x F_2(x_+). \tag{3.15}$$

The Dirac observables $\hat{p}_{(\phi)}$ and $\hat{V}|_{\phi_o}$ have the same form as in (3.8) and (3.10) but, because the transformation from b to y in the WDW theory and to x in LQC are quite different, the definition of the operator $\hat{v}$ changes:

$$\hat{v} = -\frac{2\lambda}{\sqrt{12\pi G}}(P_R(\cosh(\sqrt{12\pi G}x)i\,\partial_x)P_R + P_L(\cosh(\sqrt{12\pi G}x)i\,\partial_x)P_L). \tag{3.16}$$

This is the second difference that makes the physics of the two theories profoundly different, in spite of the fact that the states $\underline{\chi}(y,\phi)$ and $\chi(x,\phi)$ satisfy the same dynamical equation.

3.3. Physical consequences

3.3.1. Generic nature of the bounce. We have discussed that the action of $\hat{p}_\phi$ is identical in the WDW and sLQC. However, crucial differences appear in the case of the Dirac observable $\hat{V}|_\phi$ corresponding to volume. Since the right and left moving sectors decouple, let us focus on the left moving sector. On it, the expectation values of $\hat{v}|_\phi$ can be written as

$$(\underline{\chi}_L, \hat{v}|_\phi \underline{\chi}_L)_{\text{phy}} = \frac{4}{\sqrt{12\pi G}b_o} \int_{-\infty}^{\infty} dy \left|\frac{\partial\underline{\chi}_L(y,\phi)}{\partial y}\right|^2 e^{-\sqrt{12\pi G}y}. \tag{3.17}$$

Using the fact that $\underline{\chi}_L(y,\phi) = \underline{\chi}_L(y_+)$, it now follows that the expectation value of $\hat{V}|_\phi$ is given by

$$(\underline{\chi}_L, \hat{V}|_\phi \underline{\chi}_L)_{\text{phy}} = 2\pi\gamma\ell_{\text{Pl}}^2(\underline{\chi}_L, |\hat{v}|_\phi \underline{\chi}_L)_{\text{phy}} = V_* e^{\sqrt{12\pi G}\phi}, \tag{3.18}$$

where V_* is a constant determined by the state at any 'initial' time instant and is given by

$$V_* = \frac{8\pi\gamma\ell_{\text{Pl}}^2}{\sqrt{12\pi G}b_o} \int_{-\infty}^{\infty} dy_+ \left|\frac{d\underline{\chi}_L}{dy_+}\right|^2 e^{-\sqrt{12\pi G}y_+}. \tag{3.19}$$

(An analogous calculation for the right moving modes yields $(\underline{\chi}_L, \hat{V}|_{\phi}\underline{\chi}_L)_{phy} \propto e^{-\sqrt{12\pi G}\phi}$.) Hence, for the left moving modes (which correspond to an expanding universe), the expectation values $\langle \hat{V}|_{\phi}\rangle \to 0$ as $\phi \to -\infty$. Similarly, for the right moving modes, the expectation values vanish as $\phi \to \infty$. The expectation values with the left (right) moving modes diverge when ϕ approaches positive (negative) infinity. Thus, in the WDW theory, a state corresponding to a contracting universe encounters a big-crunch singularity in the future evolution, and the state corresponding to an expanding universe evolves to a big-bang singularity in the backward evolution. Note that this conclusion holds for any state in the domain of $\hat{V}|_{\phi}$. The WDW quantum cosmology is thus generically singular[9].

Let us now turn to sLQC. Now the expectation value of $\hat{v}|_{\phi}$ is given by

$$(F, \hat{v}F)_{phy} = \frac{4\lambda}{\sqrt{12\pi G}} \int_{-\infty}^{\infty} dx \left| \frac{\partial F(x_+, \phi)}{\partial x} \right|^2 \cosh(\sqrt{12\pi G}x). \qquad (3.20)$$

Therefore, equation (3.14) implies that the expectation values $\langle \hat{V}|_{\phi}\rangle$ are now given by

$$(\underline{\chi}, \hat{V}|_{\phi}\underline{\chi})_{phy} = 2\pi\gamma\ell_{Pl}^2(\underline{\chi}, |\hat{v}|_{\phi}\underline{\chi})_{phy} = V_+ e^{\sqrt{12\pi G}\phi} + V_- e^{-\sqrt{12\pi G}\phi}, \qquad (3.21)$$

where

$$V_{\pm} = \frac{4\pi\gamma\ell_{Pl}^2\lambda}{\sqrt{12\pi G}} \int_{-\infty}^{\infty} dx_+ \left| \frac{dF}{dx_+} \right|^2 e^{\mp\sqrt{12\pi G}x_+} \qquad (3.22)$$

are positive constants determined by the state at any 'initial' time instant. Unlike the WDW theory, $\langle \hat{V}|_{\phi}\rangle$ diverges in the future ($\phi \to \infty$) and in the past evolution ($\phi \to -\infty$). The minimum of the expectation values is reached at $\phi = \phi_B$ (the bounce time), determined by the initial state

$$V_{min} = 2\frac{\sqrt{V_+ V_-}}{||\chi||^2} \qquad \text{at} \qquad \phi_B = \frac{1}{2\sqrt{12\pi G}} \log \frac{V_+}{V_-}. \qquad (3.23)$$

Since V_+ and V_- are strictly positive, $\langle \hat{V}|_{\phi}\rangle$ is never zero and the big-bang/big-crunch singularities are absent. It is important to stress that the bounce occurs for arbitrary states in sLQC at a positive value of $\langle \hat{V}|_{\phi_B}\rangle$ and the resolution of classical singularity is generic. Further, the expectation values $\langle \hat{V}|_{\phi}\rangle$ are symmetric across the bounce time.

The singularity resolution in sLQC can also be understood by analyzing the expectation value of the time-dependent Dirac observable corresponding to the matter energy density,

$$\hat{\rho}|_{\phi} = \frac{1}{2}(\hat{A}|_{\phi})^2 \quad \text{where} \quad \hat{A}|_{\phi} = (\hat{V}|_{\phi})^{-1/2}\hat{p}_{\phi}(\hat{V}|_{\phi})^{-1/2}. \qquad (3.24)$$

The expectation values $\langle \hat{A}|_{\phi}\rangle$ (in any state χ) can be evaluated as

$$\langle \hat{A}|_{\phi_o}\rangle = \frac{(\chi, \hat{p}_{\phi}\chi)_{phy}}{(\chi, \hat{V}|_{\phi_o}\chi)_{phy}} = \left(\frac{3}{4\pi\gamma^2 G} \right)^{1/2} \frac{1}{\lambda} \frac{\int_{-\infty}^{\infty} dx|\partial_x F|^2}{\int_{-\infty}^{\infty} dx|\partial_x F|^2 \cosh(\sqrt{12\pi G}x)}. \qquad (3.25)$$

Clearly, these are bounded by $(3/4\pi\gamma^2 G\lambda^2)^{1/2}$. Since the state is (essentially) arbitrary, this implies that there is an upper bound on the spectrum of the energy density operator[10]:

$$\rho_{sup} = \frac{3}{8\pi\gamma^2 G\lambda^2} = \frac{\sqrt{3}}{32\pi^2\gamma^3 G^2\hbar} \approx 0.41\rho_{Pl}. \qquad (3.26)$$

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[9] This conclusion is based on the analysis of the expectation values of the Dirac observables. The same conclusion is reached if one considers consistent probabilities framework in the manner of Hartle [25] in this model. A careful analysis of histories at different times shows that even arbitrary superpositions of the left and right moving sectors do not lead to a singularity resolution in the WDW theory. The probability that a WDW universe ever encounters the singularity is unity [110, 125]. A similar analysis in sLQC reveals the probability for bounce to be unity [111]. We discuss these issues in detail in section 7.5.

[10] Another way to define the expected energy density is $\langle \hat{\rho}|_{\phi}\rangle = \langle \hat{p}_{\phi}\rangle^2/2\langle V|_{\phi}\rangle^2$. It leads to the same bound.

The value of the supremum of $\langle \hat{\rho} |_\phi \rangle$ is directly determined by the area gap and is in excellent agreement with the earlier studies based on the numerical evolution of semi-classical states [53]. As an example, for semi-classical states peaked at late times in a macroscopic universe with $\langle \hat{p}_{(\phi)} \rangle = 5000\hbar$, the density at the bound already agrees with ρ_{sup} to one part in 10^4. In the $k = 1$ case, for the universe to reach large macroscopic sizes, $\langle \hat{p}_{(\phi)} \rangle$ has to be far larger. If we use those values here, then the density at the bounce and ρ_{sup} would be indistinguishable.

3.3.2. Fluctuations. Because $\hat{p}_{(\phi)}$ is a constant of motion, its mean value and fluctuations are also time independent. For $\hat{V}|_\phi$, on the one hand, both are time dependent. In the previous subsection, we analyzed the time dependence of the expectation value. We will now summarize results on the time dependence of fluctuations $(\Delta \hat{V}|_\phi) = \langle (\hat{V}|_\phi)^2 \rangle - \langle \hat{V}|_\phi \rangle^2$. Of particular interest is the issue of whether fluctuations can grow significantly during the bounce. This issue of potential 'cosmic forgetfulness' has been analyzed from different perspectives and there has been notable controversy in the literature [54, 143–146]. For instance, the case for cosmic forgetfulness includes statements such as 'It is practically impossible to draw conclusions about fluctuations of the Universe before the Big Bang' and 'in cosmology, fluctuations before and after the Big Bang are largely independent' [143]. The case in the opposite direction is summarized in statements such as 'The universe maintains (an almost) total recall' and 'there is a strong bound on the possible relative dispersion 'on the other side' when the state is known to have, at late times, small relative dispersion in canonically conjugate variables' [54].

We will summarize three mathematical results on this issue, two of which have been obtained recently [145, 146]. For the question to be interesting, one has to assume that on one side of the bounce, say to the past, the states are sharply peaked about a classical trajectory at early times, in the sense that the relative fluctuations in both $\hat{p}_{(\phi)}$ and $\hat{V}|_\phi$ are small, and investigate if they remain small and comparable on the other side of the bounce, i.e. in the distant future.

We will begin with a powerful general result [145]. It is based on a novel scattering theory which also extends to other cosmological models which are not exactly soluble. There is no restriction on states[11] and the results are analytic, with excellent mathematical control on estimates. The focus is on the fluctuations of logarithms $\ln \hat{p}_{(\phi)}$ and $\ln \hat{V}|_\phi$ of the Dirac observables under consideration. If a state is sharply peaked so that these dispersions are very small, then they provide excellent approximations to the relative fluctuations $\Delta_R \hat{V}|_\phi := ((\Delta \hat{V}|_\phi)^{1/2})/(\langle \hat{V}|_{\phi_o} \rangle)$ and $\Delta_R \hat{p}_{(\phi)} := ((\Delta \hat{p}_{(\phi)})^{1/2})/(\langle \hat{p}_{(\phi)} \rangle)$. The analysis provides an interesting inequality relating the fluctuations of $\ln \hat{V}|_\phi$ in the distant future and in the distant past and the fluctuation in $\ln \hat{p}_{(\phi)}$ (which is constant in time):

$$|\sigma_+ - \sigma_-| \leqslant 2\sigma_\star, \tag{3.27}$$

where

$$\sigma_\pm = \left\langle \Delta \ln \frac{\hat{V}|_\phi}{2\pi \gamma \lambda \ell_{\mathrm{Pl}}^2} \right\rangle_\pm \qquad \text{and} \qquad \sigma_\star = \left\langle \Delta \ln \left(\frac{\hat{p}_{(\phi)}}{\sqrt{G}\hbar} \right) \right\rangle. \tag{3.28}$$

Here the operators have been divided by suitable constants to make them dimensionless. (Taking logarithms has a conceptual advantage in that, in the spatially non-compact case, the result is manifestly independent of the choice of the cell $\mathcal{C}$ made to construct the theory.) Thus, if we begin with a semi-classical state in the distant past well before the bounce with, say, $\sigma_- = \sigma_\star = \epsilon \ll 1$, then we are *guaranteed* that the dispersion σ_+ in the distant future after the bounce is less than 3ϵ. In this rather strong sense, semi-classicality is guaranteed

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[11] That is, results hold for all states in the domains of operators considered.

to be preserved across the bounce. Furthermore, the bound is not claimed to be optimal; the preservations could well be even stronger. However, note also that (3.27) does not rule out the possibility that σ_+ is *much smaller* than ϵ in which case the relative fluctuation in volume after the bounce would be *much smaller* than those before. On the other hand, there is no definitive result that, for semi-classical states of interest, the relative fluctuations before and after the bounce can in fact be significantly different. We are aware of only one numerical calculation [144] indicating this and it has been challenged by a more recent result [146] summarized below.

For special classes of states, one can obtain stronger results, ensuring that the fluctuations in volume in the distant past and in the distant future are comparable. Recall that, given *any* state, the expectation values $\langle \hat{V}|_{\phi_o}\rangle$ of the volume operator are symmetric around a bounce time ϕ_B. One can similarly show [54] that the expectation values $\langle \hat{V}^2|_\phi\rangle$ of the square of the volume operators are also symmetric about a time $\phi = \phi'_B$ which also depends on the choice of the state. In general, the two times are not the same. But they have been shown to be the same for generalized Gaussians [54]. From the definition of fluctuation $\Delta \hat{V}|_\phi$, it now follows that the relative fluctuations $\Delta_R \hat{V}|_\phi$ are also symmetric about $\phi = \phi_B$. Thus, for these states, the memory of fluctuations is preserved *exactly*. How big is this class of states? Recall from (3.14) that each physical state $\chi(x, \phi)$ of LQC is determined by a function $F(x)$ whose Fourier transform has support just on the positive half k-line. The generalized Gaussians are those states for which the Fourier transform is the restriction to the positive half-line of functions

$$F(k) = k^n \, \mathrm{e}^{-\frac{(k-k_o)^2}{\sigma^2}+\mathrm{i}p_o k}, \tag{3.29}$$

where n is a positive integer, the parameters k_o, σ are positive and p_o is any real number. (The factor k^n ensures that $F(k)$ is sufficiently regular at $k = 0$.) This is a 'large' set in the sense that it forms an overcomplete basis. But the result holds just for these states and *not* their superpositions.

The third result is along the same lines; it allows more general states but now the dispersions are no more exactly symmetric. In addition to the multiplicative factors k^n, the function $F(k)$ is now allowed squeezing: the parameter σ, in particular, can be complex. In this case, one bound is given by [146]

$$\left| \left. \Delta_R^+ \hat{V}\right|_\phi - \left.\Delta_R^- \hat{V}\right|_\phi \right| \leqslant \left(\frac{\kappa}{\langle \hat{p}_{(\phi)}\rangle}\right) \Delta_R^\pm \hat{V}|_\phi, \tag{3.30}$$

where the superscripts $\pm$ refer to the distant past and distant future, and κ is a constant, ~ 66 in Planck units. Since the factor $\Delta_R^\pm \hat{V}|_\phi$ appears on the right-hand side, this bound implies that, for the generalized squeezed states, the concern that the fluctuation in the future can be much smaller than that in the past (or vice versa) is not realized. The physical content of this bound is most transparent if the spatial sections are compact with $\mathbb{T}^3$ topology. To make the discussion more concrete let us suppose that, when the hypothetical universe under consideration has a radius equal to the observable radius of our own universe at the CMB time, it has the same density as our universe then had. For such a universe, $\langle \hat{p}_{(\phi)}\rangle \approx 10^{126}$ in Planck units. Thus, the coefficient on the right-hand side of (3.30) is $\sim 10^{-124}$!

To summarize, there are now two types of results on fluctuations: a general result (that holds for arbitrary states) and bounds the volume dispersion in the distant future of the bounce in terms of its value in the distant past and the dispersion in the scalar field momentum [145], and stronger bounds for special classes of states [54, 146].

3.4. Relation between the WDW theory and sLQC

As we saw in section 3.3.1, in the model under consideration, all quantum states encounter a singularity in the WDW theory but undergo a quantum bounce in sLQC. The occurrence of a bounce is a direct manifestation of the underlying quantum geometry, captured by the parameter λ, which becomes important when the spacetime curvature approaches Planck's regime. On the other hand, when the spacetime curvature is small, i.e. at large volumes for a given value of $p_{(\phi)}$, the WDW theory is an excellent approximation to sLQC. So a natural question arises: Can WDW theory be derived from sLQC in the limit $\lambda \to 0$?

To address this issue, one has to let λ vary. Let us call the resulting theory sLQC$_{(\lambda)}$. Now, a necessary condition for the WDW theory to be the limit of sLQC$_{(\lambda)}$ is that, given any state in the WDW theory, there should exist a state in sLQC$_{(\lambda)}$ such that the expectation values of the Dirac observable $\hat{V}|\phi$ in the two states remain close to each other for all ϕ, so long as λ is chosen to be sufficiently small. Let us suppose we want the predictions of the two theories to agree within an error ϵ. Then, there should exist a $\delta > 0$ such that, for all $\lambda < \delta$,

$$|\langle \hat{V}|_\phi \rangle_{(\lambda)} - \langle \hat{V}|_\phi \rangle_{(\text{wdw})}| < \epsilon \tag{3.31}$$

for all ϕ. From (3.18) and (3.21), we have

$$\langle \hat{V}|_\phi \rangle_{(\text{wdw})} = V_o e^{\sqrt{12\pi G}\phi} \qquad \text{and} \qquad \langle \hat{V}|_\phi \rangle_{(\lambda)} = V_+ e^{\sqrt{12\pi G}\phi} + V_- e^{-\sqrt{12\pi G}\phi}, \tag{3.32}$$

whence it immediately follows that if the (3.31) is to hold for all positive ϕ, then we must have $V_* = V_+$ and $V_- < \epsilon$. But since V_- is necessarily non-zero, irrespective of the choice of δ, (3.31) will be violated for a sufficiently large negative value of ϕ. Note however that for any fixed positive ϕ_o, one can choose a sufficiently small V_- so that (3.31) holds in the semi-infinite interval $(-\phi_o, \infty)$. (Similarly, if we use the right moving sector of the WDW theory, (3.31) can be made to hold in the semi-infinite intervals $(-\infty, \phi)$.) But this approximation fails to be uniform in ϕ_o whence the WDW theory cannot arise in the limit $\lambda \to 0$ of sLQC$_{(\lambda)}$. This argument is rather general and does not require the specification of a precise map between the two theories. But a useful map can be constructed using the basic ideas that underlie renormalization group flows and brings out the relation between the two theories more explicitly [76].

These considerations naturally lead us to another question: Does the limit $\lambda \to 0$ of sLQC$_{(\lambda)}$ yield a well-defined theory at all? The answer turns out to be in the negative: LQC is a fundamentally discrete theory. This is in striking contrast to the examples in 'polymer quantum mechanics' [137, 138, 147] and lattice gauge theories where a continuum limit does exist when the discreteness parameter is sent to zero. Physical reasons behind this difference are discussed in [76].

3.5. Path integral formulation

The key difference between the WDW theory and LQC is that, thanks to the quantum geometry inherited from LQG, LQC has a novel, in-built repulsive force. While it is completely negligible when curvature is less than, say, 1% of the Planck scale, it grows dramatically once curvature becomes stronger, overwhelming the classical gravitational attraction and causing a quantum bounce that resolves the big-bang singularity. From a path integral viewpoint (see, e.g., [148]), on the other hand, this stark departure from classical solutions seems rather surprising at first. For, in the path integral formulation quantum effects usually become important when the action is small, comparable to Planck's constant $\hbar$, while the Einstein–Hilbert action along classical trajectories that originate in the big bang is generically very large. Thus, there is an apparent conceptual tension. In this sub-section, we will summarize

the results of a detailed analysis [77] that has resolved this issue in $k = 0$ FLRW model. (Extension of this analysis to the $k = 1$ case is direct, see [149].)

3.5.1. Strategy. Since LQC uses a Hilbert space framework, it is most natural to return to the original derivation of path integrals, where Feynman began with the expressions of transition amplitudes in the Hamiltonian theory and *reformulated* them as an integral over all kinematically allowed paths [150]. But in non-perturbative quantum gravity, there is a twist: at a fundamental level, one deals with a constrained system without external time whence the notion of a transition amplitude does not have an *a priori* meaning. It is replaced by an *extraction amplitude*—a Green's function which extracts physical quantum states from kinematical ones and also provides the physical inner product between them (see, e.g., [102–104]). If the theory can be deparameterized, it inherits a relational time variable and then the extraction amplitude can be re-interpreted as a transition amplitude with respect to that time [103]. In LQC with a massless scalar field, we saw that a natural deparametrization is indeed available. However, more generally—e.g. if one were to introduce a potential for the scalar field—it is difficult to find a *global* time variable. Since the conceptual tension between LQC results and the path integral intuition is generic, it is best not to have to rely heavily on deparametrization. Therefore, the comparison was carried out in the timeless framework. This is also the setting of spin foams, the path integral approach to full LQG; see e.g. [99–101]. The idea then is to start with the expression of the extraction amplitude in the Hilbert space framework of LQC, cast it as a path integral, and re-examine the tension between the path integral intuition and the singularity resolution.

As we have indicated in section 2, solutions to the constraint equation, as well as inner product between them, can be obtained through a group averaging procedure [34, 48, 49]. The extraction amplitude $\mathcal{E}(v, \phi; v', \phi')$ is a Green's function that results from this averaging:

$$\mathcal{E}(v_f, \phi_f; v_i, \phi_i) := \int_{-\infty}^{\infty} d\alpha \langle v_f, \phi_f | e^{\frac{i}{\hbar} \alpha \hat{C}} | v_i, \phi_i \rangle, \tag{3.33}$$

where $\hat{C} = -\hbar^2 (\partial_\phi^2 + \Theta)$ is the full Hamiltonian constraint, α is a parameter (with dimensions $[L^{-2}]$), and the ket and the bra are eigenstates of the operators $\hat{V}$ and $\hat{\phi}$ on the kinematical Hilbert space $\mathcal{H}_{\text{kin}}^{\text{total}}$.[12] The integral averages the ket (or the bra) over the group generated by the constraint. Since the integrated operator is heuristically '$\delta(\hat{C})$,' the amplitude $\mathcal{E}(v_f, \phi_f; v_i, \phi_i)$ satisfies the constraint in both of its arguments. Consequently, it serves as a Green's function that extracts physical states $\Psi_{\text{phys}}(v, \phi)$ in $\mathcal{H}_{\text{phy}}$ from kinematical states $\Psi_{\text{kin}}(v, \phi)$ in $\mathcal{H}_{\text{kin}}^{\text{total}}$ through a convolution

$$\Psi_{\text{phys}}(v, \phi) = \sum_{v'} \int d\phi' \mathcal{E}(v, \phi; v', \phi') \Psi_{\text{kin}}(v', \phi'). \tag{3.34}$$

This is why $\mathcal{E}$ is referred to as the *extraction amplitude*. Since it is the group averaging Green's function, $\mathcal{E}$ also enables us to write the physical inner product in terms of the kinematical:

$$(\Phi_{\text{phys}}, \Psi_{\text{phys}}) := \sum_{v, v'} \int d\phi \, d\phi' \bar{\Phi}_{\text{kin}}(v, \phi) \mathcal{E}(v, \phi; v', \phi') \Psi_{\text{kin}}(v', \phi'). \tag{3.35}$$

Thus, in the 'timeless' framework without any deparametrization, all the information in the physical sector of the quantum theory is neatly encoded in the extraction amplitude $\mathcal{E}(v, p_{(\phi)}; v', p'_{(\phi)})$. Therefore, to relate the Hilbert space and path integral frameworks, it suffices to recast expression (3.33) of this amplitude as a path integral.

---

[12] Since in LQC we restrict ourselves to the 'positive frequency part' there is an implicit $\theta(\hat{p}_{(\phi)})$ factor multiplying $e^{(i/\hbar)\alpha\hat{C}}$ in (3.33) where θ is the unit step function. We do not write it explicitly just to avoid unnecessary proliferation of symbols.

3.5.2. Path integral for the extraction amplitude. Let us begin by recalling the procedure Feynman used to arrive at the path integral expression of the transition amplitude in quantum mechanics. He began with the Hamiltonian framework, wrote the unitary evolution as a composition of N infinitesimal ones, inserted a complete basis between these infinitesimal evolution operators to arrive at a 'discrete time' path integral, and finally took the limit $N \to \infty$. In the timeless framework, we need to adapt this procedure to the extraction amplitude $\mathcal{E}(\nu_f, \phi_f; \nu_i, \phi_i)$, using $e^{\frac{i}{\hbar}\alpha \hat{C}}$ in the integrand of equation (3.33) in place of the 'evolution' operator, and then performing the α integration in a final step.

More precisely, the integrand of (3.33) can be thought of as a matrix element of a *fictitious* evolution operator $e^{\frac{i}{\hbar}\alpha\hat{C}}$. One can regard $\alpha\hat{C}$ as playing the role of a (purely mathematical) Hamiltonian, the evolution time being unit. We can then decompose this fictitious evolution into N evolutions of length $\epsilon = 1/N$ and insert a complete basis at suitable intermediate steps to write the extraction amplitude as a discrete *phase space* path integral and finally take the limit $N \to \infty$ (or $\epsilon \to 0$). As is standard in the path integral literature, the result can be expressed as a formal infinite-dimensional integral

$$\mathcal{E}(\mathrm{v}_f, \phi_f; \mathrm{v}_i, \phi_i) = \int \mathrm{d}\alpha \int [\mathcal{D}\nu(T)][\mathcal{D}\mathrm{b}(T)][\mathcal{D}p_{(\phi)}(T)][\mathcal{D}\phi(T)] \, e^{\frac{i}{\hbar}S}. \tag{3.36}$$

A detailed calculation [77] shows that the action S in this expression is given by

$$S = \int_0^1 \mathrm{d}T \left(p_{(\phi)}\phi' - \frac{1}{2}\mathrm{b}\nu' - \alpha \left(p_{(\phi)}^2 - 3\pi G \nu^2 \frac{\sin^2 \lambda \mathrm{b}}{\lambda^2} \right) \right), \tag{3.37}$$

where the prime denotes the derivative with respect to the (fictitious) time T. Note that the final integration is over *all* paths in the classical phase space, *including the ones which go through the big-bang singularity*. Therefore, the tension between the Hamiltonian LQC and the path integral formulation is brought to the forefront: How can we see the singularity resolution in the path integral setting provided by (3.36)? The answer is that the paths are not weighted by the standard Einstein–Hilbert action but by a 'polymerized' version (3.37) of it which still retains the memory of the quantum geometry underlying the Hamiltonian theory. As we will see, this action is such that a path going through the classical singularity has negligible contribution whereas bouncing trajectories give the dominant contribution.

Note that the new action (3.37) retains memory of quantum geometry through the area gap λ^2. However, since λ^2 depends on $\hbar$, this means that the Einstein–Hilbert action itself has received quantum corrections. This may seem surprising at first. However, this occurs also in some familiar examples if one systematically arrives at the path integral starting from the Hilbert space framework. Perhaps the simplest such example is that of a non-relativistic particle on a curved Riemannian manifold for which the standard Hamiltonian operator is simply $\hat{H} = -(\hbar^2/2m)g^{ab}\nabla_a\nabla_b$. Quantum dynamics generated by this $\hat{H}$ can be recast in the path integral form following the Feynman procedure [150]. The transition amplitude is then given by [151]

$$\langle q, T | q', T' \rangle = \int \mathcal{D}[q(T)] \, e^{\frac{i}{\hbar}S} \tag{3.38}$$

with

$$S = \int \mathrm{d}T \left(\frac{m}{2}g_{ab}q'^a q'^b + \frac{\hbar^2}{12m}R \right), \tag{3.39}$$

where R is the scalar curvature of the metric g_{ab} and the prime denotes the derivative with respect to time T. Thus, the classical action receives a quantum correction. In particular, the extrema of this action are not the geodesics one obtains in the classical theory but rather particle trajectories in an $\hbar$-dependent potential; the two can be qualitatively different.

3.5.3.   The steepest descent approximation.   We can now use the steepest decent approximation to understand the singularity resolution in LQC from a path integral perspective. As in more familiar systems, including field theories, one expects that the extraction amplitude can be approximated as

$$\mathcal{E}(\nu_f, \phi_f; \nu_i, \phi_i) \sim (\det \delta^2 S|_0)^{-1/2}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S_0}, \tag{3.40}$$

where S_0 is the action evaluated along the trajectory extremizing the action, keeping initial and final configuration points fixed. However, there are two subtleties that need to be addressed. First, the standard WKB analysis refers to unconstrained systems and we have to adapt it to the constrained one, replacing the Schrödinger equation with the quantum constraint. This is not difficult (see, e.g., sections 3.2 and 4.2 of [26], or appendix A in [77]). However, as in the standard WKB approximation for the transition amplitude, the procedure assumes that the action that features in the path integral has no explicit $\hbar$ dependence. The second subtlety arises because, in our case, the action does depend on $\hbar$ through $\lambda \sim \sqrt{\gamma^3 \hbar}$. Therefore, to explore the correct semi-classical regime of the theory, now one has to take the limit $\hbar \to 0$, keeping $\gamma^3 \hbar$ fixed. To highlight the fact that $\gamma^3 \hbar$ is being kept constant in the limit $\hbar \to 0$, it is customary to use inverted commas while referring to the resulting 'classical' and 'semi-classical' limit. The conceptual meaning of the 'classical' limit is as follows: $\gamma \to \infty$ corresponds just to ignoring the new term in the Holst action for general relativity in comparison with the standard Palatini term [35]. What about the 'semi-classical' approximation? In this LQC model, eigenvalues of the volume operator are given by $(8\pi G \gamma \lambda \hbar) n$ where n is a non-negative integer. Therefore, in the 'semi-classical limit', the spacing between consecutive eigenvalues goes to zero and ν effectively becomes continuous as one would expect. Finally, states that are relevant in this limit have large n, just as quantum states of a rigid rotor that are relevant in the semi-classical limit have large j.

   We can now evaluate the extraction amplitude in the saddle point approximation (3.40). To calculate the Hamilton–Jacobi functional S_0, we first note that the extrema (with positive 'frequency', i.e. positive $p_{(\phi)}$) are given by

$$\nu(\phi) = \nu_{\mathrm{B}} \cosh(\sqrt{12\pi G}(\phi - \phi_{\mathrm{B}})), \tag{3.41}$$

$$\mathrm{b}(\phi) = \frac{2\,\mathrm{sign}(\nu_{\mathrm{B}})}{\gamma \lambda} \tan^{-1}(\mathrm{e}^{-\sqrt{12\pi G}(\phi - \phi_{\mathrm{B}})}), \tag{3.42}$$

where $\nu_{\mathrm{B}}, \phi_{\mathrm{B}}$ are integration constants representing values of ν, ϕ at the bounce point. As seen from the cosh dependence of the volume, these trajectories represent bouncing universes. Since $\nu(\phi)$ can vanish only on the trajectory with $\nu_{\mathrm{B}} = 0$—i.e. the trajectory $\nu(\phi) = 0$ for all ϕ—ν cannot vanish on any 'classical' trajectory which starts out away from the singularity. It is straightforward to verify that a real 'classical' solution exists for given initial and final points $(\nu_i, \phi_i;\ \nu_f, \phi_f)$ if and only if

$$\mathrm{e}^{-\sqrt{12\pi G}|\phi_f - \phi_i|} \ < \ \frac{\nu_f}{\nu_i} < \mathrm{e}^{\sqrt{12\pi G}|\phi_f - \phi_i|}. \tag{3.43}$$

For a fixed ν_i, ϕ_i, the 'classically' allowed region for ν_f, ϕ_f consists of the upper and lower quadrants formed by the dashed lines in figure 3. For ν_f, ϕ_f in these two quarters, S_0 is real and thus the amplitude (3.40) has an oscillatory behavior. Outside these regions, the action becomes imaginary and one gets an exponentially suppressed amplitude. Thus, the situation is analogous to that in quantum mechanics.

   To summarize, in the timeless framework, all the physical information is contained in the extraction amplitude which reduces to the standard transition amplitude if a global
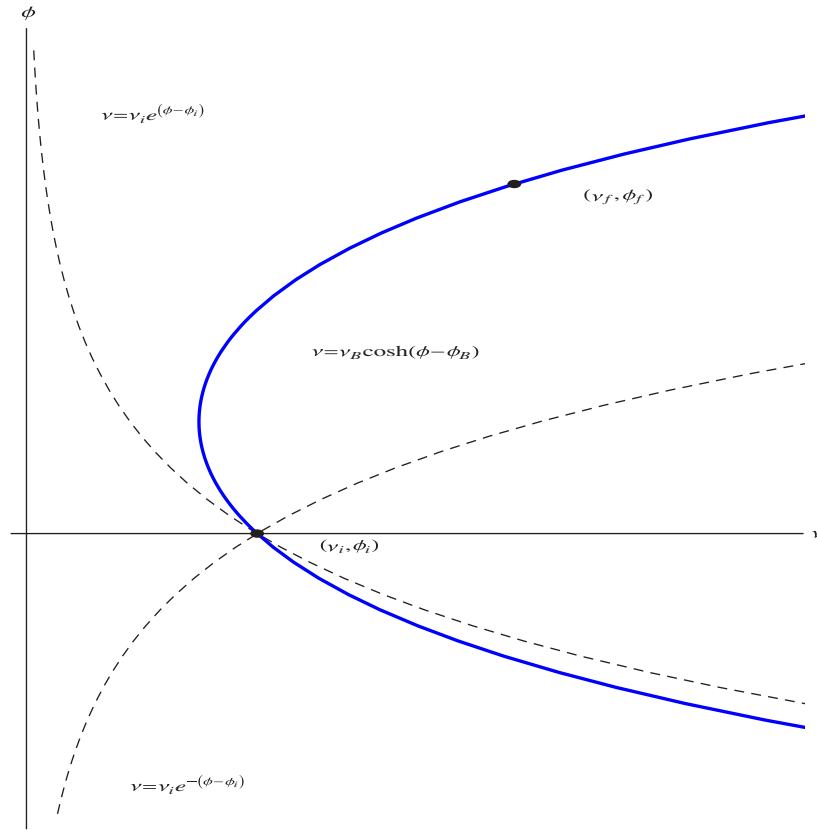
Figure 3. For fixed (ν_i, ϕ_i), the (dashed) curves $\nu_f = \nu_i\, e^{\pm\sqrt{12\pi G}(\phi_f - \phi_i)}$ divide the (ν_f, ϕ_f) plane into four regions. For a final point in the upper or lower quadrant, there always exists a real trajectory joining the given initial and final points (as exemplified by the thick line). If the final point lies in the left or right quadrant, there is no real solution matching the two points. The action becomes imaginary and one gets an exponentially suppressed amplitude.

deparametrization can be found. Following Feynman, one can start with the Hilbert space expression of the extraction amplitude and recast it as a phase space path integral. Quantum geometry effects of LQC leave their trace on the weight associated with each path. The action functional is modified. This quantum modification of the action governing path integrals is not an exceptional occurrence; the phenomenon is encountered already in the transition from Hilbert spaces to path integrals for particles moving on a curved Riemannian manifold [151]. It implies that, in the WKB approximation, the extraction amplitude is dominated by universes that undergo a bounce. Thus, from the LQC perspective, it would be incorrect to simply define the theory starting with the Einstein–Hilbert action because this procedure completely ignores the quantum nature of the underlying Riemannian geometry. For a satisfactory treatment of ultraviolet issues such as the singularity resolution, it is crucial that the calculation retains appropriate memory of this quantum nature. Indeed, this is why in the spin foam models one sums over quantum geometries, not smooth metrics.

4. Generalizations

In this section, we will retain the homogeneity assumption but consider a number of generalizations of the $k = 0$ FLRW model to include a cosmological constant, spatial curvature and anisotropies. In each case, we will encounter new conceptual issues that will require us to extend the strategy developed in section 2 to define a satisfactory Hamiltonian constraint and analyze the dynamics it leads to. While in retrospect, the necessary extensions are very natural, they were not *a priori* obvious in the course of the development of the subject. Indeed, one repeatedly found that the 'obvious' choices can lead to theories which fail to be physically viable. The fact that even in these simple models, one has to make judicious choices in the intermediate steps in arriving at the 'correct' definition of the Hamiltonian constraint suggests that the apparent freedom in defining dynamics in full LQG may in fact be highly constrained once one works out the dynamical consequences of various choices.

Since the $k = 0$ FLRW model was discussed in the last two sections in great detail, in this section we will be brief, focusing primarily on conceptual differences, new technical difficulties and their resolutions. So far, none of these models could be solved exactly. Therefore, numerical simulations are now essential. Therefore, by and large, we will now closely follow the strategies used in [53] rather than those used subsequently to show and exploit exact solvability of the $k = 0$, $\Lambda = 0$ FLRW model discussed in section 3. The numerical results bring out the fact that the singularity resolution is not tied to exact solubility.

4.1. Inclusion of spatial curvature: the k = 1 FLRW model

Although the $k = 1$ model is not observationally favored, its quantization is important for two conceptual reasons. First, it enables one to test whether the quantum bounce of the $k = 0$ case survives the inclusion of spatial curvature and, if so, whether the value of the maximum energy density is robust. The answer to these questions turns out to be in the affirmative. Second, the $k = 1$ case provides a sharper test of the infrared viability of LQC. For, if matter sources satisfy the strong energy condition, the $k = 1$ universes recollapse when its energy density reaches a value $\rho_{\min} = 3/(8\pi G a_{\max}^2)$. One can now ask if the recollapse in LQC respects this relation for universes with large $a_{\max}$. This question provides a *quantitative* criterion to test if LQC agrees with general relativity when spacetime curvature is small. Initially, there was concern that LQC may not pass this test [31]. Detailed analysis showed that it does [58].

There are also two technical reasons that warrant a careful analysis of the $k = 1$ model in LQC. The first concerns the strategy for obtaining the curvature operator using holonomies round closed loops, discussed in section 2.5. In the $k = 0$ model, one could construct the necessary closed loops following the integral curves of the fiducial triads $\mathring{e}_i^a$. In the $k = 1$ case, these triads do not commute whence their integral curves do not form closed loops. Can one still define the field strength operator? In the early stage of LQC, it was suggested [43] that one should simply add an extra edge to close the loop. In addition to being quite ad hoc, this procedure turns out not to be viable because then the loop does not enclose a well-defined area. A satisfactory strategy was developed in [58] and independently and more elegantly in [59]. The second technical point concerns numerics. In contrast to the difference operator Θ used in the $k = 1$ case, the analogous operator $\Theta_{(k=1)}$ admits a (purely) discrete spectrum, whence it is much more difficult to find its eigenvalues and eigenfunctions numerically.

4.1.1. Classical theory.

The spatial manifold M is now topologically $\mathbb{S}^3$, which can be identified with the group manifold of SU(2). We will use the Cartan–Killing form $\mathring{q}_{ab}$ on SU(2) as our fiducial metric. The fiducial volume V_o of S^3 is then given by $V_o =: \ell_o^3 = 16\pi^2$.

The fiducial triads $\mathring{e}_i^a$ on M can be taken to be the left invariant vector fields of SU(2). As before, we will denote the corresponding co-triads by $\mathring{\omega}_a^i$. The three $\mathring{e}_i^a$ and the three right invariant vector fields $\mathring{\xi}_i^a$ constitute the six Killing fields of every metric q_{ab} of the $k = 1$ model. The three vector fields in each set $\{\mathring{\xi}^i\}$ and $\{\mathring{e}_i\}$ satisfy the commutation relations of su(2) among themselves and each vector field from the first set commutes with each vector in the second.

As in the $k = 0$ case, one can solve and gauge fix the Gauss and diffeomorphism constraints and coordinatize the gravitational phase space by (c, p):

$$A_a^i = c \ell_o^{-1} \mathring{\omega}_a^i, \qquad E_i^a = p \ell_o^{-2} \sqrt{\mathring{q}} \, \mathring{e}_i^a, \tag{4.1}$$

where $\mathring{q}$ is the determinant of the fiducial metric $\mathring{q}_{ab}$. The physical metric q_{ab} is given by $q_{ab} = |p| \ell_o^{-2} \mathring{q}_{ab}$. Computing the extrinsic and intrinsic curvatures on the homogeneous slices, the curvature of the connection A_a^i turns out to be

$$F_{ab}^k = \ell_o^{-2} (c^2 - c\ell_o) \epsilon_{ij}{}^k \mathring{\omega}_a^j \mathring{\omega}_b^k. \tag{4.2}$$

The gravitational part of the Hamiltonian constraint is given by

$$
\begin{aligned}
C_{\text{grav}} &= -\gamma^{-2} \int_{\mathcal{C}} \mathrm{d}^3 x \, N (\det q)^{-1/2} \epsilon_k^{ij} E_i^a E_j^b \left[F_{ab}^k - \left(\frac{1 + \gamma^2}{4} \right) \mathring{\epsilon}_{ab}^c \mathring{\omega}_c^k \right] \\
&= -6\gamma^{-2} |p|^2 \left[\left(c - \frac{\ell_o}{2} \right)^2 + \frac{\gamma^2 \ell_o^2}{4} \right],
\end{aligned}
\tag{4.3}
$$

where in the second step, we have chosen the lapse $N = a^3 = V/V_o$ as in the quantization of the $k = 0$ model. The constraint for the spatially flat model can be obtained if we set $\ell_o = 0$. (If setting $\ell_o = 0$ seems counterintuitive, see [58] for details.)

4.1.2. Quantum theory. The kinematical part of quantization and properties of $\mathcal{H}_{\text{kin}}^{\text{grav}}$ are similar to those in the $k = 0$ case, discussed in section 2.4. The next step is to express the Hamiltonian constraint in terms of holonomies—the elementary connection variables that can be immediate quantized. In this step, an important technical subtlety arises: as explained in the beginning of this subsection, the construction of the required loops $\Box_{ij}$ is more subtle because the triad vector fields $\mathring{e}_i^a$ do not commute. However, since these left invariant vector fields do commute with the right invariant vector fields $\mathring{\xi}_i^a$, it is now natural to form closed loops $\Box_{ij}$ by following the left invariant vector fields along, say, the i direction and the right invariant ones in the j direction [58, 59]. By computing holonomies along such loops and shrinking them, as in section 2.5, so that they enclose the minimum possible physical area, one obtains the expression of the curvature operator:

$$\hat{F}_{ab}^k = \epsilon_{ij}{}^k V_o^{-\frac{2}{3}} \mathring{\omega}_a^i \mathring{\omega}_b^j \left(\frac{\sin^2 \bar{\mu}(c - \frac{\ell_o}{2})}{\bar{\mu} \ell_o} - \frac{\sin^2(\frac{\bar{\mu} \ell_o}{2})}{\bar{\mu} \ell_o} \right), \tag{4.4}$$

where $\bar{\mu} \sim 1/\sqrt{|p|}$ exactly as in equation (2.37) and where, as before, we have dropped the hats on trignometric operators for notational simplicity.

As in the $k = 0$ case, the quantum Hamiltonian constraint simplifies considerably if one works in the volume representation, i.e. with wavefunctions $\Psi(\nu, \phi)$, and uses the equality $\bar{\mu}c = \lambda b$. However, in place of operators of the form $\sin(\lambda b)$, we now have to deal with $\sin(\lambda b - \ell_o/2)$. To find its action on states $\Psi(\nu)$, we note that in the kinematical Hilbert space, we have the identity

$$\sin \left(\lambda b - \frac{\ell_o}{2} \right) \Psi(\nu) = \mathrm{e}^{\mathrm{i} \ell_o f} \sin \lambda b \, \mathrm{e}^{-\mathrm{i} \ell_o f} \Psi(\nu), \tag{4.5}$$

where

$$f = \frac{3}{8\tilde{K}} \mathrm{sgn}(\nu) \nu^{2/3} \qquad \text{with} \quad \tilde{K} := 2\pi\gamma\ell_{\mathrm{Pl}}^2. \tag{4.6}$$

Using this identity, it is straightforward to determine the action of the operator $\hat{C}_{\mathrm{grav}}$ on $\Psi(\nu)$. With the choice of lapse $N = a^3$, for the matter Hamiltonian of the massless scalar field, the total constraint $\hat{C}_H\Psi(\nu, \phi) = (\hat{C}_{\mathrm{grav}} + 16\pi G \hat{C}_{\mathrm{matt}})\Psi(\nu, \phi) = 0$ turns out to be

$$\partial_\phi^2\Psi(\nu, \phi) = -\Theta_{(k=1)}\Psi(\nu, \phi)$$
$$= -\Theta\Psi(\nu, \phi) + \frac{3\pi G}{\lambda^2}\nu\left[\sin^2\left(\frac{\lambda}{\tilde{K}\nu^{1/3}}\frac{\ell_o}{2}\right)\nu - (1+\gamma^2)\left(\frac{\lambda}{\tilde{K}}\frac{\ell_o}{2}\right)^2\nu^{1/3}\right]\Psi(\nu, \phi), \tag{4.7}$$

where Θ is the $k = 0$, second order difference operator (equation (2.45)). Thus, the quantum constraint in the $k = 1$ model turns out to be the one in the $k = 0$ model, with an additional term, due to the non-vanishing intrinsic curvature, that acts simply by multiplication. If we set $\ell_o = 0$, we recover the $k = 0$ quantum constraint. Further, as in the case of the spatially flat model, one can show that at large volumes and sufficiently smooth wavefunctions, the LQC quantum difference equation is well approximated by the WDW differential equation.

The operator $\Theta_{(k=1)}$ is self-adjoint and positive definite [59] and using group averaging, one can obtain a physical Hilbert space $\mathcal{H}_{\mathrm{phy}}$. As in the $k = 0$ model, physical states $\Psi(\nu, \phi)$ are 'positive frequency' solutions to (4.7), i.e. satisfy

$$-i\hbar\partial_\phi\Psi(\nu, \phi) = \sqrt{\Theta}\Psi(\nu, \phi) \tag{4.8}$$

and are invariant under the change of orientation of the triad, i.e. satisfy $\Psi(\nu, \phi) = \Psi(-\nu, \phi)$. The expression for the inner product turns out to be the same as equation (2.51) in the $k = 0$ model.

There is however an important difference in properties of operators $\Theta_{(k=1)}$ and Θ. In contrast to the spectrum of Θ, the spectrum of $\Theta_{(k=1)}$ is discrete and each eigenvalue is non-degenerate [59]. This feature arises because the extra term in $\Theta_{(k=1)}$ causes its eigenfunctions to decay exponentially as $|\nu|$ tends to infinity. This decay is a reflection in the quantum theory of the classical recollapse. Since Θ has discrete eigenvalues, considerable care and numerical accuracy is needed to find these eigenvalues and corresponding eigenfunctions. This makes the numerical evolution of physical states much more challenging than in the $k = 0$ model.

These technical challenges were overcome and extensive numerical simulations of closed models have been performed [58]. In figure 4, we show the results from a typical simulation. As in the numerical studies with the spatially flat model, one chooses a state peaked on a classical trajectory when the spacetime curvature is small and evolves it using the quantum constraint. Using these states and the physical inner product, one then obtains the expectation values of the Dirac observables: the momentum $\hat{p}_{(\phi)}$, and the volume at a given 'time' $\hat{V}|_\phi$. The expectation values and the relative fluctuations of $\hat{p}_{(\phi)}$ are constant throughout the evolution. The relative dispersion of $\hat{V}|_\phi$ does increase but the increase is minuscule: for a universe that undergoes a classical recollapse at ~ 1 Mpc, a state that nearly saturates the uncertainty bound *initially*, with uncertainties in $\hat{p}_{(\phi)}$ and $\hat{V}|_\phi$ spread equally, the relative dispersion in $\hat{V}|_\phi$ is still $\sim 10^{-6}$ after some 10^{50} cycles.

The expectation values of volume reveal a quantum bounce which occurs at $\rho \approx \rho_{\max}$ up to the correction terms of the order of $\ell_{\mathrm{Pl}}^2/a_{\mathrm{bounce}}^2$. For universes that grow to macroscopic sizes, the correction is totally negligible. For example, for a universe which grows to a maximum volume of 1Gpc^3, the volume at the bounce is approximately $10^{117}\ell_{\mathrm{Pl}}^3$! That the bounce occurs at such a large volume may seem surprising at first. But what matters is
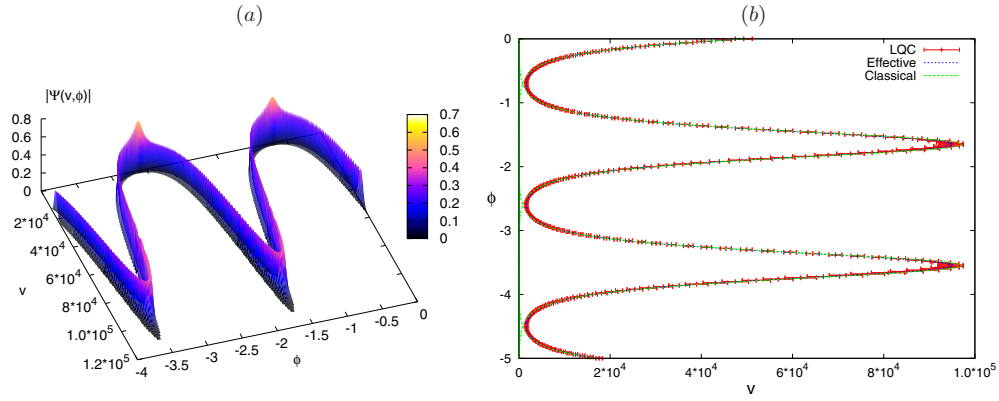
Figure 4. Quantum evolution of the $k = 1$, $\Lambda = 0$ universe. Results from a numerical evolution of a state peaked at late times with the quantum constraint are shown. (a) Plot of the wavefunction shows non-singular cycles of expansion and contraction caused by alternating quantum bounces at $\rho = \rho_{\max}$ and the classical recollapse at $\rho \approx 3/(8\pi G a_{\max}^2)$. It is evident that the peakedness properties of the state do not significantly change in consecutive cycles. (b) Expectation values of the volume observable are plotted along with the relative fluctuations and are compared with the classical trajectory and also the trajectory obtained from the effective Hamiltonian for LQC (see section 5). The classical trajectory is a good approximation to the quantum dynamics when spacetime curvature is small (large volume regime). Evolution in LQC shows a recollapse at essentially the same point as predicted by general relativity. The LQC evolution is non-singular, whereas classical trajectories undergo a big bang and a big crunch. The effective dynamics trajectory is an excellent approximation to the quantum dynamics in *all* regimes.

curvature and density and these are *always* of Planck's scale at the bounce. Thus, there is no big-bang singularity; the quantum geometry effects underlying LQC are again strong enough to cure the ultraviolet problems of general relativity. What about the infrared behavior? In this regime, there is excellent quantitative agreement with general relativity. Specifically, in general relativity $a_{\max}$, the scale factor at the classical recollapse and the density $\rho_{\min}$ are related by $\rho_{\min} = 3/(8\pi G a_{\max}^2)$. This relation holds in LQC up to corrections of the order $O(\ell_{\text{Pl}}^4/a_{\max}^4 \ell_o^4)$. For a universe that grows to the size of the observable part of our universe, this correction is *completely* negligible and agreement with general relativity is excellent.

Remarks.

(1) Using early literature in LQC, Green and Unruh [31] had expressed the concern that although the singularity is resolved the LQC universes may not undergo the recollapse predicted by general relativity at low densities and curvatures. However, the equations from the early literature they used had several important limitations. In particular, the Hamiltonian constraint was not self-adjoint and the physical Hilbert space had not even been constructed. Therefore, one could not make any reliable physical predictions. These drawbacks have been overcome and, as we just discussed, LQC passes the infrared test associated with recollapse with flying colors. Indeed, even for tiny universes that grow to a maximum size of only $25\ell_{\text{Pl}}$, general relativity is a good approximation (to one part in 10^5) in the regime in which the universe has a radius of about $10\ell_{\text{Pl}}$–$23\ell_{\text{Pl}}$! For universes that grow to a Gpc, the accuracy is one part in 10^{228}!

(2) Finally, we will comment briefly on the $k = -1$ model. The procedure used in [58] is not directly applicable because the spin connection compatible with the triad $\mathring{e}_i^a$ has off-diagonal terms. The early works [152] (and [153] where a more careful treatment

was given) suffered from some drawbacks. These can be overcome by using (non-local) operators corresponding to the connection itself (introduced in [61] and briefly discussed in section 4.4.2). However, the operator $\Theta_{(k=-1)}$ is not essentially self-adjoint. To our knowledge, the issue of possible self-adjoint extensions and robustness of the theory with respect to this ambiguity have not been studied.

4.1.3. Inverse volume corrections. For simplicity, we chose to work with harmonic time already at the classical level, by setting the lapse to be $N_\tau = a^3$. This removed all the inverse volume factors in the expression of the classical Hamiltonian constraint, prior to quantization. However, as we remarked in section 2.2, this procedure does not have a direct analog in full LQG and therefore, in the first discussions [53, 58] of the FLRW models, classical analysis was carried out with $N_t = 1$ corresponding to proper time and the scalar field was used as time only to interpret the final quantum constraint. In that procedure, to obtain the quantum Hamiltonian constraint it was essential to define operators corresponding to inverse powers p^{-n} of 'triads', p. Even if one works with $N_\tau = a^3$, these operators are also necessary to define the constraint in the Bianchi IX model and to define certain physical observables.

Since these operators have to be defined on the kinematical Hilbert space $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$, strictly speaking we should define them on wavefunctions $\Psi(p)$. However, for brevity, we will present the main idea using wavefunctions $\Psi(\nu)$ in terms of which the final constraint is written. On this $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$, $\hat{\nu}$ is a densely defined self-adjoint operator that acts by multiplication. Now, any measurable function of a self-adjoint operator is again self-adjoint. Therefore, given a function f of a real variable which is well defined everywhere on the spectrum of $\hat{\nu}$ except for a set of measure zero, $f(\hat{\nu})$ is also a self-adjoint operator on $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$. However, since $\{0\}$ is *not* a set of measure zero on the spectrum of $\hat{\nu}$—recall that the corresponding eigenvector is normalizable in $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$—inverse powers of $\hat{\nu}$ are not *a priori* well-defined self-adjoint operators. (Had the Hilbert space been $L^2(\mathbb{R})$ as in the WDW theory, there would have been no such difficulty because zero would be a point of the continuous spectrum and the set $\{0\}$ then has zero measure.)

A neat way out of this problem was proposed by Thiemann in full LQG [36, 154] and his idea has been used widely in LQC. We will illustrate the essence of this 'Thiemann trick' using the volume representation. Suppose one is interested in defining the operator corresponding to the classical function $|\nu|^{-1/2}$. Then, one first writes this function using Poisson brackets involving only *positive* powers of ν which have well-defined quantum analogs:

$$|\nu|^{-\frac{1}{2}} = \frac{i\hbar}{\lambda} (\mathrm{sgn}\,\nu)\, e^{i\lambda b} \{e^{-i\lambda b}, |\nu|^{\frac{1}{2}}\} \qquad (4.9)$$

is an exact identity on the phase space. We can now simply *define* the operator corresponding to the left-hand side by promoting the right-hand side to an operator, replacing the Poisson bracket by $1/i\hbar$ times the commutator:

$$\widehat{|\nu|^{-\frac{1}{2}}}\, \Psi(\nu) := \frac{1}{2\lambda}(\mathrm{sgn}\,\nu)(e^{i\lambda b}[e^{-i\lambda b}, |\hat{\nu}|^{\frac{1}{2}}] + [e^{-i\lambda b}, |\hat{\nu}|^{\frac{1}{2}}]\, e^{i\lambda b})\Psi(\nu), \qquad (4.10)$$

where as usual we have suppressed hats over trigonometric functions of b. (One has to treat the operator sgn ν with due care but this is not difficult.) One can readily simplify this expression using (2.42) to obtain

$$\widehat{|\nu|^{-\frac{1}{2}}}\, \Psi(\nu) = \frac{1}{2\lambda}\left||\nu + 2\lambda|^{\frac{1}{2}} - |\nu - 2\lambda|^{\frac{1}{2}}\right|\Psi(\nu). \qquad (4.11)$$

This definition has several attractive features. First, the operator is densely defined and self-adjoint. Second, every eigenvector of $\hat{v}$ is also an eigenvector of this new operator. Third, for $v \gg \lambda$, eigenvalues are approximately inverse of one another:

$$|v|^{\frac{1}{2}} \left(\frac{1}{2\lambda} ||v + 2\lambda|^{\frac{1}{2}} - |v - 2\lambda|^{\frac{1}{2}}| \right) \approx 1 + \frac{\lambda^2}{2v^2} + \frac{7\lambda^4}{4v^4} + \dots . \qquad (4.12)$$

Finally, near $v = 0$, the left-hand side of (4.11) goes as $|v|/(2\lambda)^{3/2}$ and hence vanishes at $v = 0$. Thus, the Thiemann trick provides the desired operator with the property that, away from the Planck scale, i.e. when $|v| \gg \lambda$, it resembles the naïve quantization of the classical function $1/\sqrt{|v|}$. But in the Planck regime, it provides an automatic regularization, making the operator well defined.

Since $\widehat{|v|^{-\frac{1}{2}}}$ so defined is a self-adjoint operator on $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$, its positive powers are again self-adjoint. Therefore, one can define arbitrary negative powers of $|\hat{v}|$. But the procedure has an ambiguity: we could have started out with the classical function $|v|^{-n}$ where $n \in]0, 1[$ in place of $|v|^{-1/2}$ and again constructed operators corresponding to arbitrary inverse powers of $|v|$. The results do depend on n but this is just a factor ordering ambiguity[13]. Thus, in the $k = 1$ or Bianchi IX model, one can define inverse volume factors—and, more generally, inverse scale factor operators—up to a familiar ambiguity. Numerical simulations show that if one uses states with values of $p_{(\phi)}$ that correspond to closed universes that can grow to macroscopic size, and are sharply peaked at a classical trajectory in the weak curvature region, the bounce occurs at a sufficiently large volume that these inverse scale factor corrections are completely negligible. (Typical numbers are given below.) But these effects are conceptually important to establish results that hold for all states because the inverse powers of volumes are tamed in the Planck regime: instead of growing, they die as one approaches $v = 0$!

The same considerations hold also in the $k = 0$ case if we use $\mathbb{T}^3$ spatial topology. However, in the non-compact, $\mathbb{R}^3$ case, there is a major difficulty. Now v refers to the volume of a fiducial cell C. If one rescales the cell via $C \to \beta^3 C$, for the classical function we have $|v|^{-1/2} \to \beta^{-1}|v|^{-1/2}$ while the quantum operator has a complicated rescaling behavior. Consequently, the inverse volume corrections now acquire a cell dependence and therefore do not have a direct physical meaning (see appendix B.2 of [53] for further discussion). What happens when we remove the infrared-regulator by taking the cell to fill all of $\mathbb{R}^3$? Then, the right-hand side of (4.12) goes to 1. Consequently, when the topology is $\mathbb{R}^3$, while we can construct intermediate quantum theories tied to a fiducial cell and keep track of cell dependent, inverse volume corrections at these stages, when the infrared regulator is removed to obtain the final theory, these corrections are washed out for states that are semi-classical at late times.

We will return to these corrections in sections 5 and 6.

4.2. Inclusion of the cosmological constant

In this subsection, we will incorporate the cosmological constant. Basic ideas were laid out in appendices of [53]. However, the detailed analysis revealed a number of conceptual and mathematical subtleties both in the $\Lambda < 0$ case [55] and, especially, in the $\Lambda > 0$ case [56, 57]. We will explain these features, the ensuing mathematical difficulties and the strategies that were developed to systematically address them. In the end, in all these cases, the singularity is resolved, again because of quantum geometry effects. However, in the $\Lambda > 0$ case, the analysis reveals some surprises indicating that there is probably a deeper mathematical theory that could account for other aspects of numerical results more systematically.

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[13] Also, here we have implicitly worked with the $j = 1/2$ representation of SU(2). *A priori* one could have used higher representations but then they have certain undesirable features [155, 156].

For definiteness, we will focus on the flat, i.e. $k = 0$, FLRW model, although these considerations continue to hold in the $k = 1$, closed case.

4.2.1. Negative Λ. In this sub-section, we summarize the main results of [55]. Let us begin with the classical theory. The phase space is exactly the same as in section 2.1 and we are again left with just the Hamiltonian constraint. However, as one would expect, the form of the constraint is modified because of the presence of the cosmological constant Λ. For lapse $N = 1$, in place of (2.19), we now have

$$C_H = \frac{p_{(\phi)}^2}{4\pi G |v|} - \frac{3}{4\gamma^2} b^2 |v| + \frac{\Lambda}{4} |v| \approx 0. \qquad (4.13)$$

One can easily calculate the equations of motion and eliminate proper time t in favor of the relational time defined by the scalar field ϕ. Then, the solution is given by

$$v(\phi) = \pm \frac{p_{(\phi)}}{\sqrt{\pi |\Lambda| G}} \frac{1}{\cosh \sqrt{12\pi G (\phi - \phi_o)}}, \qquad (4.14)$$

where we have assumed that the constant of motion $p_{(\phi)}$ is positive (so that the relational and proper time have the same orientation). Since the matter density $\rho = p_{(\phi)}^2 / V^2$ increases as v decreases, the form of the solution shows that the universe starts out with infinite density (i.e. a big bang) in the distant past and ends with infinite density in the distant future (i.e. a big crunch). Since $v(\phi)$ is maximum at $\phi = \phi_o$, the matter density is minimum there. In fact, (4.14) implies that total energy density, $\rho_{\text{tot}} = \rho + \rho_\Lambda$ vanishes there, where $\rho_\Lambda = \Lambda/8\pi G$ is the effective energy density in the cosmological constant term. Consequently, the Hubble parameter $\dot{v}/3v$ vanishes at $\phi = \phi_o$ and the universe undergoes a classical recollapse. Thus, the qualitative behavior of the classical solution is analogous to that in the $k = 1$ case.

Quantization is exactly the same as in section 2, except that the final quantum Hamiltonian constraint (2.45) is now modified by the addition of a cosmological constant term:

$$\partial_\phi^2 \Psi(v, \phi) = -\Theta'_\Lambda \Psi(v, \phi) := -\Theta \Psi(v, \phi) - \pi G \gamma^2 |\Lambda| v^2 \Psi(v, \phi), \qquad (4.15)$$

where Θ is the ($k = 0$, $\Lambda = 0$) difference operator defined in (2.45) and Λ is negative. As in the $\Lambda = 0$ case, one can introduce an auxiliary inner product (see (2.51)) with respect to which Θ'_Λ is a positive definite, symmetric operator on the domain $\mathcal{D}$ consisting of $\Psi(v)$ which have support on a finite number of points. This operator is essentially self-adjoint [55, 64]. The self-adjoint extension, which we again denote by Θ'_Λ, is again positive definite. However, in contrast to Θ, its spectrum is *discrete*. Furthermore, as eigenvalues increase, the difference between consecutive eigenvalues rapidly approaches a *constant, non-zero* value, determined entirely by G and Λ. This property has an important consequence. Let us consider Schrödinger states at a late time which are semi-classical, peaked at a point on a dynamical trajectory with a macroscopic value of $p_{(\phi)}$. Such states are peaked at a large eigenvalue of Θ'_Λ. Since the level spacing is approximately uniform in support of such states, their evolution yields $\Psi(v, \phi)$ which are nearly periodic in ϕ. They represent eternal, nearly cyclic quantum universes *even though we consider k = 0, spatially flat universes*. In each epoch, the universe starts out with a quantum bounce, expands till the total energy density ρ_{tot} vanishes, undergoes a classical recollapse and finally undergoes a second quantum bounce to the next epoch. At the bounce, ρ_{tot} is well approximated by $\rho_{tot} \approx 0.41 \rho_{\text{max}}$ as in the $\Lambda = 0$ case. For macroscopic $p_{(\phi)}$, the agreement between general relativity and LQC is excellent when $\rho_{\text{tot}} = \rho + \rho_\Lambda \ll \rho_{\text{max}}$; departures are significant only in the Planck regimes. In particular, as figure 5 shows, the wave packet faithfully follows the classical trajectory near the recollapse. Thus, again, LQC successfully meets the ultraviolet and infrared challenges discussed in section 1. By contrast,
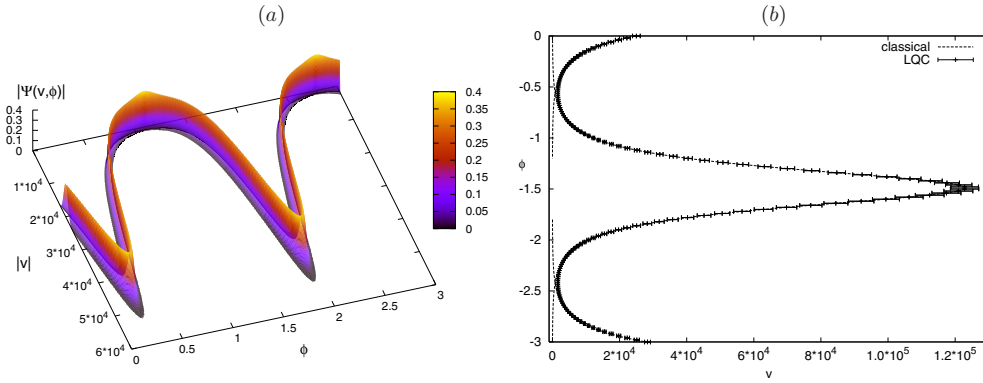
Figure 5. Quantum evolution of $k = 0$, $\Lambda < 0$ universes is contrasted with classical evolution. In the classical theory, the universe starts with a big bang, expands till the total energy density $\rho_{tot} = \rho + \Lambda/8\pi G$ vanishes and then recollapses, ending in a big-crunch singularity. In quantum theory, the big bang and the big crunch are replaced by big bounces and, for large macroscopic universes, the evolution is nearly periodic. (*a*) The evolution of a wavefunction which is sharply peaked at a point on the classical trajectory at a pre-specified late time. (*b*) Both the classical trajectory and the evolution of expectation values of the volume operator. It is clear that the LQC predictions for recollapse agree very well with those of classical general relativity but there is a significant difference in Planck regimes.

as in the $\Lambda = 0$ case, the WDW theory fails to resolve the big-bang and the big-crunch singularities.

Remark. Because the level spacing between the eigenvalues of Θ'_Λ is not exactly periodic, there is a slight spread in the wavefunction from one epoch to the next. However, this dispersion is *extremely* small. For a macroscopic universe with $\Lambda = 10^{-120} m_{Pl}^2$, the initially minute dispersion doubles only after 10^{70} cycles [55]!

4.2.2. Positive Λ. While the change from a continuous spectrum of Θ to a discrete one for Θ'_Λ had interesting ramifications, a positive cosmological constant introduces further novel features which are much more striking [56, 57].[14] Let us begin with the classical theory. While the Hamiltonian constraint is again given by (4.13), because of the flip of the sign of Λ the solutions

$$\text{v}(\phi) = \pm \frac{p_{(\phi)}}{\sqrt{\pi |\Lambda| G}} \frac{1}{\sinh \sqrt{12\pi G(\phi - \phi_o)}} \qquad (4.16)$$

are qualitatively different. First, we have the well-known consequence: because the effective energy density ρ_Λ associated with the cosmological constant is now positive, the universe expands out to infinite volume. The second and less well-known difference is associated with the use of the scalar field as a relational time variable. As in the $\Lambda < 0$ case, each solution starts out with a big bang in the distant past, expands, but reaches *infinite* proper time t at a *finite* value ϕ_o of the scalar field. At $\phi = \phi_o$, the physical volume V of the fiducial cell reaches infinity (whence ρ_{matt} goes to zero). This means that if we use the lapse tailored to the use of the scalar field as the time variable, in contrast to the $\Lambda < 0$ case, the Hamiltonian vector field on the phase space is *incomplete*. This raises the question of whether the phase space can be

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[14] Most of section 4.2.2 is based on a preprint [56]. We are grateful to Tomasz Pawlowski for his permission to quote these results here.

extended to continue dynamics beyond $\phi = \phi_o$. From a physical viewpoint, it is instructive to consider matter density ρ. Along any dynamical trajectory, its evolution is given by

$$\rho(\phi) = \frac{\Lambda}{8\pi G} \sinh^2(\sqrt{12\pi G}(\phi - \phi_o)) \tag{4.17}$$

which clearly admits an analytical extension beyond $\phi = \phi_o$. It suggests that from the viewpoint of the Hamiltonian theory, it is natural to extend the phase space. While this is not essential in the classical theory—one can just stop the evolution at $\phi = \phi_o$ since proper time and the volume of the fiducial cell become infinite there—we will find that it is instructive to carry out the extension from a quantum perspective.

For the analytical extension, let us introduce a new variable θ given by

$$\alpha \tan \theta = 2\pi \gamma \ell_{\mathrm{Pl}}^2 \nu \tag{4.18}$$

(the right-hand side is just the oriented volume of the fiducial cell and the constant α has been introduced for dimensional reasons). To begin with, $\theta \in]0, \pi/2[$, the big bang corresponding to $\theta = 0$, and $\phi = \phi_o$ to $\theta = \pi/2$. The Friedmann equation written in terms of θ (in place of the scale factor) and ϕ (in place of proper time) is analytic in ϕ: $(\partial_\phi \theta)^2 = \sin^2 \theta \; [(4\alpha^2 \Lambda / 3 p_{(\phi)}^2) \sin^2 \theta + 12\pi G \cos^2 \theta]$ and so is the solution:

$$\tan \theta(\phi) = \left[\frac{\sqrt{4\pi G} \, p_{(\phi)}}{\alpha \sqrt{\Lambda}} \frac{1}{\sinh(\sqrt{12\pi G}(\phi - \phi_o))} \right] \tag{4.19}$$

Therefore, it is natural to extend the range of θ to $\theta \in]0, \pi[$. On this extended phase space, dynamical trajectories start with a big bang at $\phi = -\infty$ expand out till $\phi = \phi_o$ where ρ goes to zero and then contract into a big-crunch singularity at $\phi = \infty$.

Let us now consider the quantum theory. The Hamiltonian constraint is given by

$$\partial_\phi^2 \Psi(\nu, \phi) = -\Theta_\Lambda \, \Psi(\nu, \phi) := -\Theta \, \Psi(\nu, \phi) + \pi G \gamma^2 \Lambda \nu^2 \Psi(\nu, \phi), \tag{4.20}$$

where Λ is now positive. The operator Θ_Λ is again symmetric on the dense domain $\mathcal{D}$ consisting of $\Psi(\nu)$ with support on a finite number of points. However, unlike the operator Θ_Λ' of (4.15), Θ_Λ fails to be essentially self-adjoint [57]. This is *not* a peculiarity of LQC; essential self-adjointness fails also in the WDW theory. From a mathematical physics perspective, this is not surprising. Already in non-relativistic quantum mechanics, if the potential is such that the particle reaches infinity in finite time, the corresponding Hamiltonian fails to be essentially self-adjoint in the Schrödinger theory.

The freedom in the choice of self-adjoint extensions has been discussed in detail in [57]. For any choice of extension, the spectrum of Θ_Λ is discrete but the precise eigenvalues depend on the choice of the extension. However, for large eigenvalues of Θ_Λ, the spacing between consecutive eigenvalues rapidly approaches a constant value which depends only on the cosmological constant and not on the choice of the self-adjoint extension. In this respect, the situation is the same as in the $\Lambda < 0$ case.

We are most interested in the case when $1/\Lambda \gg \ell_{\mathrm{Pl}}^2$ so that the effective energy density $\rho_\Lambda = \Lambda/8\pi G$ in the cosmological constant is small compared to the Planck scale, i.e. $\rho_\Lambda \ll \rho_{\max}$. Furthermore, we are interested in the quantum evolution of states which are initially sharply peaked at a point in the classical phase space at which $p_{(\phi)}^2 \gg m_{\mathrm{Pl}} \ell_{\mathrm{Pl}}^3$ and $\rho \ll \rho_{\max}$. For these states, numerical simulations show that the evolution is robust, largely independent of the choice of the self-adjoint extension. Because these states are sharply peaked at a large eigenvalue of $\hat{p}_{(\phi)}^2$, as in the $\Lambda < 0$ the evolution is nearly periodic. In each epoch, the universe starts at a quantum bounce, expands till the *matter* density ρ goes to zero (and the volume of the fiducial cell goes to infinity), and then 'recollapses'. This contracting phase ends with a quantum bounce to the next epoch. At each bounce, the *total* energy density
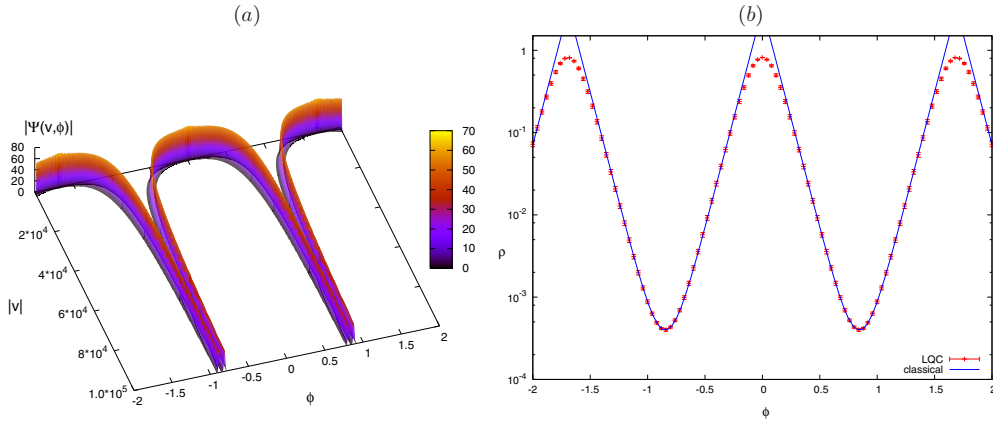
Figure 6. Quantum evolution of $k = 0$, $\Lambda > 0$ universes is contrasted with classical evolution. In the classical theory, the universe starts with a big bang, and expands till the matter energy density ρ_{matt} vanishes. This occurs at a finite value of the scalar field time and the solution can be analytically continued. In quantum theory, for *any* choice of the self-adjoint extension of Θ_λ, the big bang and the big crunch are replaced by big bounces and, for large macroscopic universes, the evolution is nearly periodic. (*a*) The evolution of wavefunction which are sharply peaked at a point on the classical trajectory with $p_{(\phi)} = 5000 m_{Pl}^2$ at a pre-specified late time. (*b*) Both the classical trajectory and the evolution of the expectation value of the *total* density operator. It is clear that there are very significant differences in the Planck regime but excellent agreement away from it.

$\rho + \rho_\Lambda$ is extremely well approximated by $\rho_{max} \approx 0.41 \rho_{Pl}$ as in sections 2 and 3. As figure 6 shows, in the region where $\rho \ll \rho_{max}$, the trajectory is well approximated by the analytical extension (4.19) of the classical solution. In this sense, LQC again successfully resolves the ultraviolet difficulties of the classical theory without departing from it in the infrared regime. Again, by contrast, the WDW theory fails to resolve the singularities.

Remarks.

(1) In the classical theory, the volume of the fiducial cell becomes infinite at a finite value, $\phi = \phi_o$, of the relational time. In the quantum theory, if a wave-packet were to start in a 'tame regime' well away from the big bang and follow this trajectory, it would also reach infinite volume at a finite value of ϕ. However, if dynamics is unitary—as it indeed is for each choice of the self-adjoint extension of Θ_Λ—the wavefunction has a well defined evolution all the way to $\phi = \infty$. If it is to remain semi-classical, one can ask what trajectory it would be peaked on beyond $\phi = \phi_o$. As we have remarked above, the trajectory is just the analytical extension (4.19) of the classical solution we began with. Thus, if quantum dynamics is to be unitary, semi-classical considerations imply that an extension of the classical phase space is inevitable.

(2) It is however quite surprising that the evolution of such semi-classical states is largely independent of the self-adjoint extension chosen. Part of the reason may be that the classical trajectories could be extended simply by invoking analyticity. This 'natural' avenue enables one to bypass the complicated issue of choosing boundary conditions to select the continuation of the classical solution. But the precise reason behind the numerically observed robustness of the quantum evolution is far from being clear and further exploration may well lead one to an interesting set of results on sufficient conditions

under which inequivalent self-adjoint extensions yield nearly equivalent evolutions of semi-classical states.

(3) The Friedmann equation of classical general relativity implies that, at very late times when the dominant contribution to ρ_{tot} comes from the cosmological constant term, the Hubble parameter has the behavior $H = \dot{a}/a \sim \sqrt{\Lambda}$, whence the connection variable $c \sim \dot{a} \sim \sqrt{\Lambda} V^{1/3}$. Thus, in striking contrast to the $\Lambda = 0$ case, c *grows* at late times even when Λ and hence the spacetime curvature is very small (in Planck units). Therefore, had $\bar{\mu}$ been a constant, say μ_o, as in [45], at late times we would have $\mu_o c \sim \sqrt{\Lambda} V^{1/3}$. Thus, in the μ_o-LQC, $\sin \mu_o c / \mu_o$ does not approximate c at late times whence the theory has large deviations from general relativity in the low curvature regime. Thus, the correct infrared limit of LQC is quite non-trivial: the fact that the field strength operator was obtained using the specific form $\bar{\mu} \sim 1/\sqrt{|\mu|} \sim 1/V^{1/3}$ of $\bar{\mu}$ plays a key role.

4.3. Inclusion of an inflaton with a quadratic potential

At the quantum bounce, the Hubble parameter H necessarily vanishes and $\dot{H}$ is positive. Therefore, immediately after the bounce, $\dot{H}$ continues to be positive, i.e. there is a phase of superinflation. At first there was a hope that this phase of accelerated expansion may be an adequate substitute for the inflationary epoch [40]. However, this turned out not to be the case because, in the absence of a potential for the scalar field, the superinflation phase is too short lived. Thus, to compare predictions of LQC with those of the standard inflationary paradigms, an inflaton potential appears to be essential at this stage of our understanding.

Effective equations discussed in section 5 imply that a sufficient condition for the quantum geometry corrections to resolve the big-bang singularity is only that the inflaton potential be bounded below [83]. For full LQC, while the general strategy necessary to construct the theory is clear for this class of potentials, to handle technical issues and carry our numerical simulations, it has been necessary to fix a potential. The simplest choice is a quadratic mass term for the inflaton. This potential has been widely used in inflationary scenarios and is compatible with the 7 year WMAP data [83, 157]. Therefore, in this sub-section, we will focus on the quadratic potential and summarize the status of incorporating it in full LQC (i.e. beyond the effective theory)[15].

Let us begin with a general remark before entering the detailed discussion. Recall first that the powerful singularity theorems [158] of Penrose, Hawking and others strongly suggest that if matter satisfies standard energy conditions, the big-bang singularity is inevitable in general relativistic cosmology. However, the inflaton with a quadratic potential violates the strong energy condition. Therefore, in the initial discussions of inflationary scenarios, one could hope that the presence of such an inflaton by itself may suffice to avoid the initial singularity. However, Borde, Guth and Vilenkin [159] subsequently proved a new singularity theorem with the novel feature that it does not use an energy condition and is thus not tied to general relativity. This important result is sometimes paraphrased to imply that there is no escape from the big bang[16]. This is not the case: since the new theorem was motivated by ideas from eternal inflation, it assumes that the expansion of the universe is always positive and this assumption is violated in all bouncing scenarios, including LQC. Thus, the LQC resolution of the big-bang singularity can evade the original singularity theorems of general relativity [158]

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[15] Most of section 4.3 is based on a preprint [67]. We are grateful to Tomasz Pawlowski for his permission to quote these results here.

[16] For example, the following remark in [160] is sometimes interpreted to imply that the big-bang singularity is inevitable also in quantum gravity [161]: 'With the proof now in place, cosmologists can no longer hide behind the possibility of a past-eternal universe. There is no escape: they have to face the problem of a cosmic beginning.'

even when matter satisfies *all* energy conditions because Einstein's equations are modified due to quantum gravity effects, *and* it evades the more recent singularity theorem of [159] which is not tied to Einstein's equations because the LQC universe has a contracting phase in the past.

With these preliminaries out of the way, let us return to the Hamiltonian constraint in the $k = 0$ FLRW model with an inflaton in a quadratic potential, $V(\phi) = (1/2)m^2\phi^2$:

$$C_H = \frac{p_{(\phi)}^2}{4\pi G|v|} - \frac{3}{4}b^2|v| + \frac{1}{4}(\Lambda + 4\pi Gm^2\phi^2)|v| \approx 0. \qquad (4.21)$$

Note that the potential term is positive and naturally grouped with the cosmological constant. As a consequence there is considerable conceptual similarity between the two cases. Phenomenologically, the contribution due to the cosmological constant term is completely negligible in the early universe. However, to emphasize the partial similarity with section 4.2.2, we will not ignore it in this section. In particular, the structure of the quantum Hamiltonian constraint is similar to that in section 4.2.2:

$$\partial_\phi^2 \Psi(v, \phi) = -\Theta_{(m)} \Psi(v, \phi) := -(\Theta - \pi G\gamma^2(\Lambda + 4\pi Gm^2\phi^2)v^2)\Psi(v, \phi). \qquad (4.22)$$

There are, however, two qualitative differences between this constraint and those of other models we have considered so far. First, since we have a non-trivial potential, $p_{(\phi)}$ is no longer conserved in the classical theory and ϕ fails to be globally monotonic in solutions to field equations. Therefore, ϕ no longer serves as a *global* internal time variable. Nonetheless, we can regard ϕ as a *local* internal time around the putative big bounce because, in the effective theory, ϕ is indeed monotonic in a sufficiently long interval containing the bounce. The second important difference is that $\Theta_{(m)}$ carries an explicit 'time' dependence because of the ϕ^2 term. Therefore, we cannot repeat the procedure of taking the positive square-root to pass to a first order differential equation: $-i\partial_\phi \Psi = \sqrt{|\Theta|} \Psi$ is not admissible because the square of this equation is no longer equivalent to the original constraint (4.22). Consequently, even locally we do not have a convenient deparametrization of the Hamiltonian constraint; now the group averaging strategy becomes crucial. For any fixed value of ϕ, since the form of $\Theta_{(m)}$ is the same as that of Θ_Λ with a positive cosmological constant (see (4.20)), it again fails to be essentially self-adjoint. Furthermore, now we have freedom in choosing a self-adjoint extension for each value of ϕ. Given a choice of these extensions, we can again carry out group averaging and arrive at the physical sector of the theory. Because we do not have a global clock, we are forced to use a genuine generalization of ordinary quantum mechanics: one can make well-defined relational statements but these have connotations of 'time evolution' only locally. Thus, in any given physical sector, we still have a meaningful generalized quantum mechanics [25] and it is feasible to carry out a detailed analysis using a consistent histories approach described in section 7.5. However, the question of the detailed relation between theories that emerge from different choices of self-adjoint extensions is still quite open. Numerical studies indicate that for states which are semi-classical, there is again robustness. But, as we will now discuss, the scope of these studies is much more limited than that in the case of a positive cosmological constant [56].

Suppose we make a choice of self-adjoint extensions and thus fix a physical sector. The question is whether the expectations based on effective equations are borne out in this quantum theory. Since the model is not exactly soluble, we have to take recourse to numerics. Because physical states must in particular satisfy (4.22), we can again use this equation to probe dynamics. However, the ϕ-dependence of $\Theta_{(m)}$ introduces a number of technical subtleties.

To discuss these, it is simplest to work with states $\Psi(\mathrm{b}, \phi)$, i.e. use the representation in which the variable b conjugate to ν is diagonal. Then, one finds that the Hamiltonian constraint (4.22) is hyperbolic in the region $\mathcal{R}$ of the (b, ϕ) space given by

$$\frac{\sin^2 \lambda \mathrm{b}}{\gamma^2 \lambda^2} - \frac{8\pi G}{3} m^2 \phi^2 - \frac{2\Lambda}{3} > 0 \qquad (4.23)$$

(and the choice of a self-adjoint extension of $\Theta_{(m)}$ corresponds to a choice of a boundary condition at the boundary of $\mathcal{R}$). So far, numerics have been feasible as long as the wavefunction remains in the region $\mathcal{R}$. Now, we are interested in states which are sharply peaked on a general relativity trajectory in the regime in which general relativity is an excellent approximation to LQC. The question is: if we evolve them backward in time using (4.22), do they remain sharply peaked on the corresponding solution of effective equations across the bounce? To answer this question, we need a sufficiently long 'time' interval so that the state can evolve from a density of, say, $\rho = 10^{-4} \rho_{\max}$ where general relativity is a good approximation to the putative bounce point and then beyond. For the wavefunction to remain in $\mathcal{R}$ during this evolution, the initial state has to be sharply peaked at a phase space point at which the kinetic energy is greater than the potential energy (because in general relativity $\sin^2 \lambda \mathrm{b}/\gamma^2 \lambda^2 = H^2 = (8\pi G/3)\, \rho$ and we need (4.23) to hold). Numerical simulations show that such LQC wavefunctions do remain sharply peaked on the effective trajectory. In particular, they exhibit a bounce.

In summary, to incorporate an inflationary potential in the effective theory is rather straightforward [83]. To incorporate it in full LQC, one has to resolve several technical problems. So far, the issue of the dependence of the theory on the choice of the self-adjoint extension of $\Theta_{(m)}$ has remained largely open on the analytical side. On the numerical side, simulations have been carried out for quantum states which are initially sharply peaked at a phase space point at which the total energy density is low enough for general relativity to be an excellent approximation and, in addition, the kinetic energy density is greater than potential. In these cases, in a backward evolution, wavefunctions continue to remain sharply peaked on effective trajectories at and beyond the bounce, independently of the choice of the self-adjoint extension. If we were to allow greater potential energy initially, with current techniques one can evolve the wavefunctions over a more limited range of ϕ. Therefore, in this case, one would have to start the evolution in a regime in which general relativity fails to be a good approximation. But it should be possible to adapt the initial state to a trajectory given by effective equations of LQC and check if, in the backward evolution, it continues to remain peaked on that trajectory all the way to the bounce and beyond.

4.4. Inclusion of anisotropies

In isotropic models, the Weyl curvature vanishes identically while in the presence of anisotropies it does not. Therefore, there are many more curvature invariants and in general relativity they diverge at different rates at the big bang, making the singularity structure more sophisticated. Indeed, according the BKL conjecture [10, 11], the behavior of the gravitational field as one approaches generic space-like singularities can be largely understood using homogeneous but anisotropic models. This makes the question of singularity resolution in these models conceptually important.

We will be interested in homogeneous models in which the group of isometries acts simply and transitively on spatial slices. Then, the spatial slices can be identified with three-dimensional Lie-groups which were classified by Bianchi. Let us denote the three Killing fields by $\mathring{\xi}_i^a$ and write their commutation relations as $[\mathring{\xi}_i, \mathring{\xi}_j] = \mathring{C}_{ij}^k \mathring{\xi}_k$. The metrics under

consideration admit orthonormal triads $\mathring{e}_i^a$ such that $[\mathring{\xi}_i, \mathring{e}_j] = 0$. As before the fiducial spatial metric $\mathring{q}_{ab}$ on the manifold is determined by the dual co-triad $\mathring{\omega}_i^a$ via $\mathring{q}_{ab} := q_{ij}\mathring{\omega}_a^i\mathring{\omega}_b^j$.

Bianchi I, II and IX models have been discussed in LQC. In the Bianchi I case, the group is Abelian whence the spatial topology is $\mathbb{R}^3$ or $\mathbb{T}^3$. In the Bianchi II model, the isometry group is that of two translations and a rotation on a null 2-plane. So we can choose the Killing fields such that all the structure constants vanish *except* $\mathring{C}_{23}^1 = -\mathring{C}_{32}^1 =: \tilde{\alpha}$. The spatial topology is now $\mathbb{R}^3$. In the Bianchi IX model, the isometry group is SU(2) and the spatial topology is $\mathbb{S}^3$. In the isotropic limit, the Bianchi I model reduces to the $k = 0$ FLRW model and the Bianchi IX to the $k = 1$ FLRW model.

While the general strategy is the same as that in section 2, its implementation turns out to be surprisingly non-trivial. In the Bianchi I model for example, first investigations [162, 163] attempted to use the obvious generalization of the expression of the field strength operator in the isotropic case discussed in section 2.5. However, this procedure led to unphysical results—problems with the infrared limit and dependence of the final theory on the initial choice of cell—reminiscent of what happened in the μ_o-scheme in the isotropic case [164, 165]. As in the isotropic case, one has to start anew and implement in the model ideas from full LQG [3] step by step rather than attempting to extend just the final result. This procedure led us to a satisfactory Hamiltonian constraint which, however, was difficult to use. Therefore, a second new idea was needed to write its expression in a closed form and then a third input was needed to render the final expression to a manageable form. The resulting quantum theory is then free of the limitations of [162, 163]. The singularity is indeed resolved in the quantum theory and, furthermore, there is again a universal bound on energy density ρ and the shear scalar in the effective theory. Interestingly, the bound on ρ agrees with the $\rho_{\max}$ obtained in the isotropic cases.

In this construction, the field strength could be expressed in terms of the holonomy around a suitable plaquette whose edges are the integral curves of $\mathring{e}_i^a$. This procedure turns out not to be viable in the Bianchi II model because we now have both, spatial curvature *and* anisotropies. Therefore, a new strategy was introduced in [61]: construct non-local operators corresponding to connections themselves and use them to define the field strength. This procedure is a generalization of the one used in the Bianchi I case in which it reproduces the same answer as in [3]. Fortunately, these inputs seem to suffice for more complicated models. In particular, the LQC of the Bianchi IX model does not need further conceptual tools. In both Bianchi II and IX models, the singularity is resolved. In the Bianchi II and IX models, in the effective theory there is again a bound on ρ but there is no analytical argument that it is optimal (see section 5.5).

In this section, there is no summation over repeated indices which are all covariant or all contravariant; summation is understood only if there is a contraction between a covariant and a contravariant index.

4.4.1. Bianchi I model. The spacetime metrics of the Bianchi I model can be written as

$$ds^2 = -N^2\, d\tau^2 + a_1^2\, dx_1^2 + a_2^2\, dx_2^2 + a_3^2\, dx_3^2, . \tag{4.24}$$

If the spatial topology is $\mathbb{R}^3$, we again have to fix a fiducial cell $\mathcal{C}$. We will take its edges to lie along the integral curves of the fiducial triads $\mathring{e}_i^a$ with coordinate lengths L_1, L_2, L_3 so that the fiducial volume of $\mathcal{C}$ is $V_o = L_1 L_2 L_3$. In terms of these background structures, the gravitational connection and conjugate (density weighted) triad can be written as

$$A_a^i = c^i (L^i)^{-1} \mathring{\omega}_a^i, \qquad \text{and} \quad E_i^a = p_i L_i V_o^{-1} \sqrt{\mathring{q}}\, \mathring{e}_i^a, \tag{4.25}$$

where $\mathring{q}$ is again the determinant of $\mathring{q}_{ab}$. Thus, the gravitational phase space is now six-dimensional, parameterized by (c^i, p_i). The physical volume V of $\mathcal{C}$ is given by $V^2 = p_1 p_2 p_3$ and the triad components are related to the directional scale factors in the metric via

$$p_1 = \varepsilon_1 L_2 L_3 |a_2 a_3|, \qquad p_2 = \varepsilon_2 L_1 L_3 |a_1 a_3|, \qquad p_3 = \varepsilon_3 L_1 L_2 |a_1 a_2|, \qquad (4.26)$$

where $\varepsilon_i \pm 1$ depending on whether E_i^a is parallel or antiparallel to $\mathring{e}_i^a$.

Next, let us discuss the effect of changing the fiducial structures under which physics must be invariant. As in the case of the isotropic model (discussed in section 2.1.2), (c^i, p_i) are unchanged under the rescaling of coordinates x^i. However, in contrast to the isotropic case, we now have the freedom of performing a different rescaling of the cell along each direction, $L_i \to \beta_i L_i$, under which the fiducial volume transforms as $V_o \to \beta_1 \beta_2 \beta_3 V_o$. The connection and triad components are not invariant under this transformation. For example, the $i = 1$ components transform as $c_1 \to \beta_1 c_1$ and $p_1 \to \beta_2 \beta_3 p_1$ (and similarly for other components). This fact will be important in what follows.

As in the isotropic model, our canonical variables A_a^i, E_i^a; $\phi, p_{(\phi)}$ automatically satisfy the Gauss and the diffeomorphism constraints and we are only left with the Hamiltonian constraint

$$\int_{\mathcal{C}} N \left(-\frac{1}{16\pi G \gamma^2} \frac{\epsilon_k^{ij} E_i^a E_j^b F_{ab}^k}{\sqrt{q}} + \frac{p_{(\phi)}^2}{2} \frac{\sqrt{q}}{V^2} \right) \mathrm{d}^3 x \approx 0. \qquad (4.27)$$

Let us again use the lapse $N = a_1 a_2 a_3$ adapted to harmonic time and the expressions (4.25) of A_a^i, E_i^a. Then, the Hamiltonian constraint becomes

$$C_H^{(I)} = \frac{p_{(\phi)}^2}{2} - \frac{1}{8\pi G \gamma^2} (c_1 p_1 c_2 p_2 + c_3 p_3 c_1 p_1 + c_2 p_2 c_3 p_3) \approx 0. \qquad (4.28)$$

Hamilton's equations for the triads lead to a generalization of the Friedman equation

$$H^2 = \frac{8\pi G}{3} \rho + \frac{\Sigma^2}{a^6}, \qquad (4.29)$$

where a is the mean scale factor defined as $a := (a_1 a_2 a_3)^{1/3}$, H refers to the mean Hubble rate and Σ^2 represents shear

$$\Sigma^2 = \frac{a^6}{18} ((H_1 - H_2)^2 + (H_2 - H_3)^2 + (H_3 - H_1)^2). \qquad (4.30)$$

Equation (4.29) quantifies that the energy density in gravitational waves captured in the anisotropic shears $(H_i - H_j)$. From the dynamical equations, it follows that if the matter has vanishing anisotropic stress—so ρ depends on scalar factors a_i only through a—then Σ^2 is a constant of motion in general relativity.

Construction of quantum kinematics closely follows the isotropic case. The elementary variables are the triads p_i and the holonomies $h_i^{(\ell)}$ of the connection A_a^i along edges parallel to the three-axis x_i whose edge lengths with respect to the fiducial metric are ℓL_i. The holonomies can be expressed entirely in terms of almost periodic functions of the connection of the form $\exp(i\ell c_i)$. These, along with the triads, are promoted to operators in the kinematical Hilbert space $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$. In the triad representation, with states represented as $\Psi(p_1, p_2, p_3)$, the $\hat{p}_i$ act by multiplication and the $\exp(i\ell c_i)$ by displacement of the argument of Ψ, exactly as in the isotropic case. Finally, we have to incorporate the fact that physics should be invariant under a reversal of triad orientation. Therefore, the physical states satisfy $\Psi(p_1, p_2, p_3) = \Psi(|p_1|, |p_2|, |p_3|)$, whence it suffices to consider the restrictions of states to the positive octant, $(p_1, p_2, p_3) \geqslant 0$. Individual operators in a calculation may not leave this sector invariant but their physically relevant combinations do.

To discuss dynamics, we have to construct the Hamiltonian constraint operator. As in the isotropic case, we cannot directly use the reduced form (4.28) because it contains c_i while only $\exp i\ell c_i$ are well-defined operators on $\mathcal{H}_{\text{kin}}^{\text{grav}}$. Therefore, we have to return to (4.27) and seek guidance from full LQG. As before, the key problem is that of defining the quantum operator $\hat{F}_{ab}{}^i$ and, as in section 2.5.1, it can be expressed as the holonomy operator associated with suitable loops $\Box_{ij}$. Since the triads $\mathring{e}_i^a$ commute, we can form the required plaquettes $\Box_{ij}$ by moving along their integral curves. The question is: What should the lengths $\bar{\mu}_i$ of individual segments be? Because of anisotropy, $\bar{\mu}_i$ can change from one direction to another. Therefore, we have to return to the semi-heuristic relation between LQG and LQC and extend the procedure of section 2.5.2 to allow for anisotropies. When this is done, one finds that $\bar{\mu}$ is replaced by [3]

$$\bar{\mu}_1 = \lambda \sqrt{\frac{|p_1|}{|p_2 p_3|}}, \qquad \bar{\mu}_2 = \lambda \sqrt{\frac{|p_2|}{|p_1 p_3|}}, \qquad \text{and} \qquad \bar{\mu}_3 = \lambda \sqrt{\frac{|p_3|}{|p_1 p_2|}}. \qquad (4.31)$$

In the isotropic case, $p_i = p$ and one recovers equation (2.37)[17].

The final field strength operator (2.38) of the isotropic case is now replaced by

$$\hat{F}_{ab}{}^k = \epsilon_{ij}{}^k \left(\frac{\sin \bar{\mu}c}{\bar{\mu}L} \mathring{\omega}_a \right)^i \left(\frac{\sin \bar{\mu}c}{\bar{\mu}L} \mathring{\omega}_a \right)^j \qquad \text{where} \qquad \left(\frac{\sin \bar{\mu}c}{\bar{\mu}L} \mathring{\omega}_a \right)^i = \frac{\sin \bar{\mu}^i c^i}{\bar{\mu}^i L^i} \mathring{\omega}_a^i \qquad (4.32)$$

(where there is no summation over i in the second expression). From their definition, it follows that the $\bar{\mu}_i$'s are invariant with respect to the rescaling of the coordinates but transform non-trivially under the allowed scalings of the fiducial edge lengths: $\bar{\mu}_i \to \beta_i^{-1} \bar{\mu}_i$. Since, the connection components transform as $c_i \to \beta_i c_i$, the crucial term $\sin(\bar{\mu}_i c_i)$ in (4.32) is invariant under *both* the rescalings. This is the key to ensuring that the physics of the final theory is insensitive to the initial choice of the infrared regulator, the fiducial cell.

However, because $\bar{\mu}_1$, say, depends also on p_2 and p_3, the operator $\sin(\bar{\mu}_1 c_1)$ is rather complicated and seems totally unmanageable at first. However, it becomes manageable if one carries out two transformations [3]:

(i) Work with the 'square-roots' l_i of p_i, given by $p_i = (\text{sgn}\, l_i)\left(4\pi\gamma\lambda\ell_{\text{Pl}}^2\right)^{2/3} l_i^2$. Then, one can write the action of $\sin(\bar{\mu}_i c_i)$ explicitly, using, e.g.,

$$e^{\pm i\bar{\mu}_1 c_1} \Psi(l_1, l_2, l_3) = \Psi\left(l_1 \pm \frac{\text{sgn}(l_1)}{l_2 l_3}, l_2, l_3\right). \qquad (4.33)$$

But the action of the resulting constraint operator is not transparent because it mixes all arguments in the wavefunction and does not have any resemblance to constraint (2.45) we encountered in the isotropic case.

(ii) A further transformation overcomes these drawbacks. Set

$$v = 2(l_1 l_2 l_3) \quad \text{so that} \quad V = 2\pi\gamma\lambda^2\ell_{\text{Pl}}|v| \qquad (4.34)$$

as in the isotropic case. Since V is the physical volume of the cell, v is related to the variable ν we used in the isotropic case via $v = \nu\ell_{\text{Pl}}/\lambda^2$. This constant rescaling makes v dimensionless and simplifies the constraint. The key idea, now, is to work with wavefunctions $\Psi(l_1, l_2, v)$ in place of $\Psi(l_1, l_2, l_3)$.

Then, the final quantum constraint has the familiar form

$$\partial_\phi^2 \Psi(l_1, l_2, v; \phi) = -\Theta_{(I)} \Psi(l_1, l_2, v; \phi) \qquad (4.35)$$

---

[17] In the early work on the Bianchi I model in LQC [162, 163], a shortcut was taken by using instead the 'obvious' generalization $\bar{\mu}_i = \lambda/\sqrt{|p_i|}$ of the isotropic $\bar{\mu}$. As we explained at the beginning of this subsection, this led to a theory that is not viable. The lesson again is that, when new conceptual issues arise, one should not guess the solution from that in the simpler cases but rather start *ab initio* and seek guidance from full LQG.

and, because of the reflection symmetry—which is preserved by the Hamiltonian constraint—it suffices to specify $(\Theta_{(I)}\Psi)(l_1, l_2, v)$ only for (l_1, l_2, v) in the positive octant (where l_1, l_2, v are all non-negative). We then have

$$\Theta_{(I)}\Psi(l_1, l_2, v; \phi) = \frac{\pi G\hbar^2}{8} v^{1/2}\big[(v+2)(v+4)^{1/2}\Psi_4^+(l_1, l_2, v) - (v+2)v^{1/2}\Psi_0^+(l_1, l_2, v; \phi)$$
$$- (v-2)v^{1/2}\Psi_0^-(l_1, l_2, v; \phi) + (v-2)|v-4|^{1/2}\Psi_4^-(l_1, l_2, v; \phi)\big] \qquad (4.36)$$

with

$$\Psi_4^{\pm}(l_1, l_2, v; \phi) = \Psi\left(\frac{v\pm 4}{v\pm 2}l_1, \frac{v\pm 2}{v}l_2, v\pm 4\right) + \Psi\left(\frac{v\pm 4}{v\pm 2}l_1, l_2, v\pm 4\right)$$
$$+ \Psi\left(\frac{v\pm 2}{v}l_1, \frac{v\pm 4}{v\pm 2}l_2, v\pm 4\right) + \Psi\left(\frac{v\pm 2}{v}l_1, l_2, v\pm 4\right)$$
$$+ \Psi\left(l_1, \frac{v\pm 2}{v}l_2, v\pm 4\right) + \Psi\left(l_1, \frac{v\pm 4}{v\pm 2}l_2, v\pm 4\right) \qquad (4.37)$$

and

$$\Psi_0^{\pm}(l_1, l_2, v; \phi) = \Psi\left(\frac{v\pm 2}{v}l_1, \frac{v}{v\pm 2}l_2, v\right) + \Psi\left(\frac{v\pm 2}{v}l_1, l_2, v\right)$$
$$+ \Psi\left(\frac{v}{v\pm 2}l_1, \frac{v\pm 2}{v}l_2, v\right) + \Psi\left(\frac{v}{v\pm 2}l_1, l_2, v\right)$$
$$+ \Psi\left(l_1, \frac{v}{v\pm 2}l_2, v\right) + \Psi\left(l_1, \frac{v\pm 2}{v}l_2, v\right). \qquad (4.38)$$

The physical Hilbert space and the Dirac observables—the scalar field momentum $\hat{p}_{(\phi)}$ which is a constant of motion, and the relational geometrical observables, the volume $\hat{V}|_\phi$ and anisotropies $\hat{l}_1|_\phi$ and $\hat{l}_2|_\phi$—can be introduced on $\mathcal{H}_{\text{phy}}$ exactly as in the isotropic case.

Equation (4.35) is still rather complicated and further simplifications have been made to make it easier to carry out numerical simulations [166]. But it is possible to draw some general conclusions already from this equation. Note first that it suffices to specify the wavefunctions on the positive octant since their values on the rest of the (l_1, l_3, v) space is determined by the symmetry requirement $\Psi(l_1, l_2, v) = \Psi(|l_1|, |l_2|, |v|)$. As in the isotropic case, the evolution preserves the space of wavefunctions which have supported only the lattices $v = 4n$ and $v = \epsilon + 2n$ if $\epsilon \neq 0$ in the positive octant. Each of these sectors is also preserved by a complete set of Dirac observables, $\hat{p}_{(\phi)}$, volume $\hat{v}|_\phi$ and anisotropies $\hat{l}_1|_\phi$ and $\hat{l}_2|_\phi$. Therefore, we can focus just on one sector. Let us consider the $\epsilon = 0$ sector since it contains the classical singularity. From the functional dependence on v of various terms in the quantum constraint, it is straightforward to deduce that the classical singularity is decoupled from the quantum evolution: if initially the wavefunction vanishes on points with $v = 0$, it continues to vanish there. Because the physical wavefunctions have support only on points $v = 4n$, it follows that the matter density, for example, can never diverge as the state evolves in the internal time. In this sense, the singularity is resolved by constraint (4.35). In the limit, $l_1, l_2, v \gg 1$, and assuming that the wavefunction is slowly varying, one can show that the discrete quantum constraint (4.35) approximates the differential quantum constraint in the WDW theory. However, in the Planck regime, there is significant difference because the singularity is not resolved in the WDW theory. Further details on dynamics are discussed in section 5.4 using effective equations.

Remarks.

(1) As mentioned in section 1.3, in the cosmology circles, there has been a general concern about bouncing models (see, e.g., [23]) which may be summarized as follows. Because the universe contracts prior to the bounce, the shear anisotropies grow and, in general relativity, this growth leads to the 'Mixmaster chaotic behavior'. Therefore, the singularity resolution through a bounce realized in isotropic models may not survive in the presence of anisotropies. How does LQC avoid this potential problem? It does so because of the in-built corrections to Einstein's equations that result from quantum geometry. When the dynamics of the model is constructed by paying full attention to full LQG, as was done in [3], the effective repulsive force created by these quantum corrections is far more subtle than what a perturbation theory around an isotropic bouncing model may suggest. There is not a single bounce but many: each time a shear potential enters the Planck regime the new repulsive force dilutes it avoiding the formation of a singularity. (See section 5.4.)

(2) The Bianchi I model also enables one to address a conceptual issue: Does quantization commute with symmetry reduction? There is a general concern that if one first quantizes a system and then carries out a symmetry reduction by freezing the unwanted degrees of freedom, the resulting quantum theory of the symmetry-reduced subsystem will not in general be quite different from the one obtained by first freezing the unwanted degrees of freedom classically and then carrying out quantization [2]. If one takes the Bianchi I model as the larger system and the isotropic FLRW model as the symmetry-reduced system, this procedure would have made us restrict the wavefunctions $\Psi(l_1, l_2, v)$ of the Bianchi I model to configurations $l_1 = l_2 = (v/2)^{1/3}$ and ask if this quantum theory agrees with that of the FLRW model. The answer, as suggested in [2], is in the negative: the Bianchi I dynamics (4.35) does not even leave this subspace invariant! However, instead of freezing the anisotropies to zero, if one integrates them out, one finds that the Bianchi I quantum constraint operator projects down *exactly* to the $k = 0$ FLRW quantum constraint operator [3]. The exact agreement in this specific calculation is presumably an artifact of the simplicity of the models. In more general situations, one would expect only an approximate agreement. But the result does bring out the fact that the issue of comparing a quantum theory with its symmetry-reduced version is somewhat subtle and contrary to one's first instincts that the dynamics of the reduced system may correctly capture appropriate physics.

(3) The treatment we summarized here uses the scalar field as a relational time variable. LQC of *vacuum* Bianchi models has also been studied using one of the triad components *or* its conjugate momentum as internal time [6, 60]. This work is conceptually important in that time has emerged from a geometrical variable *and* one can compare quantum theories with two different notions of time for the same classical model. However, technically it used the $\bar{\mu}_i$ given in the early work [162, 163]. For conceptual issues concerning time, this is not a significant limitation. Nonetheless, for completeness, it is desirable to redo that analysis with the 'correct' $\bar{\mu}_i$.

4.4.2. Bianchi II and Bianchi IX models. In this subsection, we summarize the quantization of Bianchi II and Bianchi IX spacetimes [61, 62]. Since the Bianchi I model was discussed in some detail here we will focus just on the main differences from that case.

The Bianchi II model is the simplest example of a spacetime with anisotropies *and* a non-zero spatial curvature. Since the topology of spatial slices is now $\mathbb{R}^3$, one must introduce a fiducial cell $\mathcal{C}$ to construct a Hamiltonian (or Lagrangian) framework. We will use the same notation for fiducial structures as in our discussion of the Bianchi I model. By contrast, the

spatial manifold in the Bianchi IX case is compact with topology $\mathbb{S}^3$. Therefore, a cell is *not* needed. In this case, we will use the same notation as in the $k = 1$ model discussed in section 4.1. In particular, the volume V_o of $\mathbb{S}^3$ defined by the fiducial metric $\mathring{q}_{ab}$ will be written as $V_o =: \ell_o^3 (= 16\pi^2)$.

As before, we will use a lapse N geared to the harmonic time already in the classical theory. Then, the structure of the Hamiltonian constraint is similar to that in the Bianchi I model but there are important correction terms. For the Bianchi II model, we have

$$C_H^{(II)} = C_H^{(I)} - \frac{1}{8\pi G \gamma^2}\left[\alpha \varepsilon p_2 p_3 c_1 - (1 + \gamma^2)\left(\frac{\alpha p_2 p_3}{2 p_1}\right)^2\right], \tag{4.39}$$

where $C_H^{(I)}$ is the Bianchi I constraint (4.28), $\varepsilon = \pm 1$ is determined by the orientation of the triads and we have appropriately rescaled $\tilde{\alpha} := \mathring{C}_{23}^1$ and set $\alpha := (L_2 L_3 / L_1)\tilde{\alpha}$. Note that in the limit $\alpha \to 0$, the spatial curvature in the Bianchi II model vanishes and we recover the Bianchi I constraint (4.28). Similarly, for the Bianchi IX model one obtains

$$C_H^{(IX)} = C_H^{(I)} - \frac{1}{8\pi G \gamma^2}\left[\ell_o \varepsilon (p_1 p_2 c_3 + p_2 p_3 c_1 + p_3 p_1 c_2) + \frac{\ell_o^2}{4}(1 + \gamma^2)\right.$$
$$\left. \times \left(2(p_1^2 + p_2^2 + p_3^2) - \left(\frac{p_1 p_2}{p_3}\right)^2 - \left(\frac{p_2 p_3}{p_1}\right)^2 - \left(\frac{p_3 p_1}{p_2}\right)^2\right)\right]. \tag{4.40}$$

The Bianchi I constraint (4.28) is now recovered in the limit $\alpha \to 0$. In the isotropic truncation $c_i = c$ and $p_i = p$, one recovers the classical constraint for the $k = 1$ FLRW model. A detailed examination shows that in both cases, the Hamiltonian constraint is left invariant under the change of orientation of triads, and is simply rescaled by an overall factor of $(\beta_1 \beta_2 \beta_3)^2$ under the rescaling of the fiducial cell $\mathcal{C}$ by $L_i \to \beta_i L_i$. The equations of motion are unaffected under both these operations.

The kinematics of LQC is identical to that in the Bianchi I model. However, an important subtlety occurs already in the Bianchi II case when we try to write a field strength operator using holonomies around closed loops. First, the triads $\mathring{e}_i^a$ do not commute. Therefore, we cannot use them directly to form closed loops. We already encountered this difficulty in the $k = 1$ FLRW model, where we could construct the desired loops by moving alternately along integral curves of $\mathring{e}_i^a$ and of the Killing vectors $\mathring{\xi}_i^a i$. One can repeat the same procedure but because the Bianchi II geometry is *anisotropic*, the resulting holonomy fails to be an almost periodic function of c_i whence the field strength operator so constructed is not well defined on $\mathcal{H}_{\text{kin}}^{\text{grav}}$! One can try to enlarge $\mathcal{H}_{\text{kin}}^{\text{grav}}$ but then the analysis quickly becomes as complicated as full LQG. This problem was overcome [61] by a further extension of the strategy which is again motivated by the procedure used in full LQG [36, 154]: define a non-local *connection operator* in terms of holonomies along open segments

$$\hat{A}_a \equiv \hat{A}_a^i \tau_i = \sum_k \frac{1}{2\ell_k L_k}\left(h_k^{\ell_k} - \left(h_k^{\ell_k}\right)^{-1}\right), \tag{4.41}$$

where the length of the segment along the kth direction, as measured by the fiducial metric, is $\ell_k L_k$ and τ_i is the basis in su(2) introduced in section 1.5. In full LQG, because of diffeomorphism invariance, the length of the segment does not matter. In LQC, we have gauge fixed the diffeomorphism constraint through our parametrization (4.25) of the phase space variables A_a^i, E_i^a in terms of (c^i, p_i). Therefore, we have to specify the three ℓ_k. Here one seeks guidance from the Bianchi I model: the requirement that one should reproduce exactly the same field strength operator as before fixes ℓ_k to be $\ell_k = 2\bar{\mu}_k$, where $\bar{\mu}_k$ is given by

(4.31)[18]. Once this is done, it is straightforward to write the quantum Hamiltonian constraint both in the Bianchi II and the Bianchi IX cases in the form $\partial_\phi^2 \Psi = \Theta_{(II)} \Psi$ and $\partial_\phi^2 \Psi = \Theta_{(IX)} \Psi$. The operators $\Theta_{(II)}$ and $\Theta_{(IX)}$ contain terms in addition to those in Θ_I. They also have the correct behavior under rescalings of the fiducial cell $\mathcal{C}$ and under the reversal of orientation. They disappear in the limit $\alpha \to 0$ in the Bianchi I case and $\ell_o \to 0$ in the Bianchi IX case ensuring that these theories are viable generalizations of the Bianchi I LQC. The physical Hilbert space and a complete set of Dirac observables can be constructed in a straightforward fashion. Finally, in both these cases, the big-bang singularity is resolved in the same sense as in the Bianchi I model: the singular sector (i.e. states in $\mathcal{H}_{\mathrm{kin}}^{\mathrm{total}}$ which have support on configurations $v = 0$) decouples entirely from the regular sector so that states which start having no support on the singular sector cannot acquire a singular component.

There are nonetheless significant open issues. First, the question of essential self-adjointness of $\Theta_{(I)}$, $\Theta_{(II)}$ and $\Theta_{(IX)}$ is open and it is important to settle it. For example, if $\Theta_{(IX)}$ turns out to be essentially self-adjoint, then quantum dynamics would be unambiguous and unitary in spite of the chaotic behavior in general relativity. This would not be surprising because that behavior refers to the approach to singularity which is completely resolved in LQC. Second, while there have been advances in extracting physics from effective equations in these models (see section 5.5), further work is needed in the Bianchi II and especially Bianchi IX models. It is even more important to perform numerical simulations in exact LQC to check that the effective equations continue to capture the essence of the quantum physics also in this model. These simulations should also shed new light on the relevance of the BKL conjecture for LQG.

5. Effective dynamics and phenomenological implications

In this section, we summarize the new physics that has emerged from the modified Friedmann dynamics derived from the effective Hamiltonian constraint, $C_H^{\mathrm{(eff)}}$. This constraint is defined on the classical phase space but incorporates the leading quantum corrections of LQC. Therefore, it enables one to extract the salient features of LQC dynamics using just differential equations, without having to refer to Hilbert spaces and operators.

The section is organized as follows. In section 5.1, we outline the conceptual frameworks that have been used to obtain $C_H^{\mathrm{(eff)}}$. In section 5.2, we derive the modified Einstein's equations using this effective Hamiltonian constraint and discuss key features of the new physics they lead to. These include a phase of super-inflation occurring for matter obeying the null energy condition when $\rho_{\max}/2 < \rho < \rho_{\max}$, and generic resolution of strong singularities in the LQC for the isotropic model. In section 5.3, we consider effective LQC dynamics using a scalar field in a quadratic potential. A key question is whether an inflationary phase that is compatible with the 7 year WMAP data will be seen generically in LQC or if it results only after (perhaps extreme) fine tuning. We first discuss the subtleties associated with measures that are needed to answer this question quantitatively and then summarize the result that 'almost all' data at the bounce surface evolve into solutions that meet this phase at some time during evolution. In section 5.4, we discuss the effective dynamics for Bianchi I models and summarize the results on the viability of ekpyrotic/cyclic models in LQC. We conclude with a brief summary of various other applications in section 5.5.

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[18] Just as in the older treatment of the Bianchi I model, one fixed $\bar{\mu}_k$ by using an 'obvious' generalization of the successful FLRW strategy [162, 163]; here, one may be tempted to use a similar 'shortcut' and set $\ell_k = \lambda \bar{\mu}_k$, say. But this strategy is not viable because it does not yield the correct field strength operator even in the FLRW model [167].

5.1. Effective Hamiltonian constraint

In LQC, the effective Hamiltonian constraint has been derived using two approaches: the embedding method [78–80] and the truncation method [168, 169]. The former is analogous to the variational technique, often used in non-relativistic quantum mechanics, where a skillful combination of science and art often leads to results which approximate the full answer with surprising accuracy. The latter is in the spirit of the order by order perturbation theory, which has the merit of being a more systematic procedure. Both of these approaches are based on a geometrical formulation of quantum mechanics (see, e.g., [170, 171]). The basic idea is to cast quantum mechanics in the language of symplectic geometry, i.e. the same framework that one uses in the phase space description of classical systems. One starts by treating the space of quantum states as a phase space, Γ_Q, where the symplectic form, Ω_Q, is given by the imaginary part of the Hermitian inner product on the Hilbert space $\mathcal{H}$. The framework has two surprising features. First, there is an interesting interplay between the commutators between operators on $\mathcal{H}$ and the Poisson bracket defined by Ω_Q. Given any Hermitian operator $\hat{A}$ on $\mathcal{H}$, we obtain a smooth real function $\bar{A}$ on Γ_Q by taking its (normalized) expectation value on quantum states. Then, one has an *exact* identity on Γ_Q:

$$\text{If} \quad [\hat{A}, \hat{B}] = \hat{C}, \qquad \text{then} \quad \bar{C} = i\hbar \Omega_Q^{\alpha\beta} \partial_\alpha \bar{A} \partial_\beta \bar{B} \equiv i\hbar \{\bar{A}, \bar{B}\}_Q \tag{5.1}$$

for all Hermitian operators $\hat{A}$, $\hat{B}$. Here, to be explicit, we have chosen an index notation for $\mathcal{H}$, denoting a quantum state Ψ as a vector Ψ^α. Note that this is not the usual 'Dirac quantization prescription' because $\hat{A}$ and $\hat{B}$ are arbitrary Hermitian operators and the identity holds on the infinite-dimensional Γ_Q rather than on the finite-dimensional classical phase space Γ. The second surprising fact relates unitary flows generated by arbitrary Hermitian operators $\hat{H}$ on $\mathcal{H}$ and the Hamiltonian flow generated by the function $\bar{H}$ on Γ_Q. The two flows coincide:

$$(\hat{H}\Psi)^\alpha = i\hbar \left(\Omega_Q^{\alpha\beta} \partial_\beta \bar{H}\right)\big|_\Psi. \tag{5.2}$$

From this perspective, quantum mechanics can be regarded as a special case of classical mechanics! Special, because Γ_Q carries, in addition to the symplectic structure, a Riemannian metric determined by the real part of the inner product (whence Γ_Q is a Kähler space). The metric is needed to formulate the standard measurement theory but is not important for our present considerations.

Because the space of quantum states is now regarded as a phase space (Γ_Q, Ω_Q), one can hope to relate it to the classical phase space (Γ, Ω) and transfer information about quantum dynamics, formulated on (Γ_Q, Ω_Q), to the classical phase space (Γ, Ω). This procedure gives the effective equations on (Γ, Ω) that capture the leading order quantum corrections. We will first describe the truncation method, and then focus on the embedding approach which will be used extensively in the rest of this section.

Let us suppose that the classical phase space Γ is labeled by canonical pairs (q_i, p_i). In quantum theory, we have the analogous operators $\hat{q}_i, \hat{p}_i$ on $\mathcal{H}$. Now, any state $\Psi \in \mathcal{H}$ is completely determined by the specification of the expectation values of all polynomials constructed from $\hat{q}_i, \hat{p}_j$. Therefore, one can introduce a convenient coordinate system on the infinite-dimensional quantum phase space Γ_Q, using the expectation values $(\bar{q}_i, \bar{p}_i)$ of the basic canonical pairs, expectation values $(\overline{q_i^2}, \overline{p_i^2}, \overline{q_i p_j})$ of their quadratic combinations and so on for higher order polynomials. The expectation values $(\bar{q}_i, \bar{p}_i)$ are in 1–1 correspondence with the canonical coordinates (q_i, p_i) on the classical phase space Γ and the rest represent 'higher moments'. The Hamiltonian flow on Γ_Q determined by the exact unitary dynamics on $\mathcal{H}$ provides evolution equations for $(\bar{q}_i, \bar{p}_i)$ and all the moments. These are infinitely many, coupled, nonlinear differential equations dictating the time-evolution on $\bar{\Gamma}_Q$ and the full set is

equivalent to the exact quantum dynamics. The idea is to truncate this set at some suitably low order, solve the equations, and obtain solutions $\bar{q}_i(t)$, $\bar{p}_i(t)$ which include the leading order quantum corrections to the classical evolution. The method is systematic in that, in principle, one can go to any order one pleases. But in practice it is difficult to go beyond the second or the third order and there is no *a priori* control on the truncation error. This framework makes it possible to calculate the 'back-reaction' of the evolution of higher moments on the desired evolution of expectation values $\bar{q}_i(t)$, $\bar{p}_i(t)$. However, in general, these effects are sensitive to the initial choice of state.

In the embedding approach, one seeks an embedding $\Gamma \rightarrow \bar{\Gamma}_Q \subset \Gamma_Q$ of the finite-dimensional classical phase space Γ into the infinite-dimensional quantum phase space Γ_Q that is well suited to capture quantum dynamics. To define $\bar{\Gamma}_Q$, for any given point $\gamma^o \in \Gamma$, where $\gamma^o = (q_i^o, p_i^o)$, one has to find a quantum state Ψ_{γ^o} and these Ψ_{γ^o} are to constitute $\bar{\Gamma}_Q$. The first requirement is kinematic: the embedding should be such that $q_i = \langle \Psi_{\gamma^o} \hat{q}_i \Psi_{\gamma^o} \rangle =: \bar{q}^i$ and $p_i = \langle \Psi_{\gamma^o} \hat{p}_i \Psi_{\gamma^o} \rangle =: \bar{p}^i$. An elementary example of the required embedding is given by coherent states: fix a set of parameters σ_i and let Ψ_γ^o be a coherent state peaked at (q_i^o, p_i^o) with uncertainty in q_i given by σ_i. The second condition that the embedding captures quantum dynamics is highly non-trivial. It requires that the *quantum Hamiltonian vector field should be approximately tangential to* $\bar{\Gamma}_Q$. If this condition is achieved, one can simply project the exact quantum Hamiltonian vector field on to $\bar{\Gamma}_Q$ and obtain an approximate quantum evolution there. But since $\bar{\Gamma}_Q$ is naturally isomorphic to Γ, this gives us a flow on the classical phase space *representing the desired quantum corrected evolution*. For a harmonic oscillator, one can make the Hamiltonian vector field on Γ_Q *exactly* tangential to $\bar{\Gamma}_Q$ simply by choosing σ^i as the appropriate function of the frequencies, masses and $\hbar$. Then there are no quantum corrections to the classical equations; peaks of the chosen coherent states will follow the exact classical trajectories. For a general Hamiltonian, the dynamical condition is difficult to achieve. But if one does succeed in finding an embedding such that the quantum Hamiltonian vector field is indeed very nearly tangential to $\bar{\Gamma}_Q$, the resulting effective equations can approximate the quantum evolution very well. The error can be estimated by calculating the ratio of the component of the Hamiltonian vector field orthogonal to $\bar{\Gamma}_Q$ to the component that is tangential. The method is not systematic: it is an 'art' to find a good embedding.

In LQC, the existence of such an embedding has been established in various cases. This method was first used in the context of the so-called μ_o quantization [45] to obtain quantum-corrected effective Hamiltonian constraint for a dust-filled universe [78]. In the improved $\bar{\mu}$ quantization [53], the embedding approach has been used to derive the quantum-corrected Einstein's equations for the FLRW model with a massless scalar field [79], and for arbitrary matter with a constant equation of state [80].

Let us now discuss the underlying conditions on the choice of judicious states for the case of a massless scalar field. One starts with Gaussian states with spreads σ and $\sigma_{(\phi)}$ in the gravitational and matter sectors, respectively, peaked at suitable points of the classical phase space. In terms of the variables introduced in section 2, satisfaction of the dynamical condition requires that the following inequalities hold simultaneously: (i) $v \gg \ell_{Pl}$, (ii) $\lambda b \ll 1$, (iii) $\Delta b/b \ll 1$ and $\Delta v/v \ll 1$, and (iv) $\Delta\phi/\phi \ll 1$ and $\Delta p_{(\phi)}/p_{(\phi)} \ll 1$. The first two inequalities are meant to incorporate the idea that the initial state is peaked at large volumes where the gravitational field is weak, and the last two inequalities are to ensure that the state is sharply peaked with small relative fluctuations in both gravitational and matter degrees of freedom. Some of these inequalities turn out to be mutually competing and *a priori* cannot be satisfied without additional constraints of the basic fields (because, for example, we only have two widths σ and $\sigma_{(\phi)}$, and four uncertainties Δv, Δb, $\Delta\phi$ and $\Delta p_{(\phi)}$). But a careful examination shows that the additional constraint is very weak [79]: $p_{(\phi)} \gg 3\hbar$, which is *very*

easily satisfied if the state is to represent a universe that approximately resembles ours, say in the CMB epoch.

Using such states, we then compute the expectation values of the quantum constraint operator $\hat{C}_H$, and of the operators corresponding to the basic phase space variables. The latter define the embedding of Γ into $\bar{\Gamma}_Q$. One can check that, within the systematic approximations made, the quantum Hamiltonian vector field is indeed tangential to the image $\bar{\Gamma}_Q$ of Γ in Γ_Q. The generator of the Hamiltonian flow provides us with the effective Hamiltonian constraint

$$C_H^{(\text{eff})} = -\frac{3\hbar}{4\gamma\lambda^2}\nu \sin^2(\lambda b) + \mathcal{H}_{\text{matt}} + O(\sigma^2, \nu^{-2}, \sigma^{-2}\nu^{-2}), \tag{5.3}$$

where $\mathcal{H}_{\text{matt}}$ denotes the matter Hamiltonian.

Approximations used in the derivation of the effective Hamiltonian constraint seem to break down before the evolution encounters the Planck regime [79]. Nonetheless, as often happens in theoretical physics, the resulting effective equations have turned out to be applicable well beyond the domain in which they were first derived. In particular, they predict a value for the density at the bounce that is in exact agreement with the supremum of the spectrum of the density operator in sLQC [76], discussed in section 3. Furthermore, extensive numerical simulations have shown that solutions to the effective equations track the exact quantum evolution of the peaks of those wavefunctions that start out being semi-classical in the low curvature regime. This behavior has been verified in the $k = 0$ models with or without a cosmological constant, with an inflaton in a quadratic potential, and in the $k = 1$ model discussed in sections 2–4.

5.2. Effective dynamics in LQC: key features

Using the effective Hamiltonian constraint, it is straightforward to obtain the modified Einstein's equations in LQC. These equations lead to two important predictions: (i) existence of a phase of super-inflation following the bounce [172], and (ii) a generic resolution of strong curvature singularities [173]. To analyze the physical implications of the effective Hamiltonian constraint (5.3), we consider matter with an equation of state satisfying $P = P(\rho)$, where P denotes the pressure. We further restrict the attention to the leading part in (5.3) and drop the correction terms proportional to the fluctuations. For brevity, we only discuss the case of the spatially flat model. Extensions to spatially curved models are discussed in [58, 152, 174].

5.2.1. Modified Einstein equations and super-inflation.
The strategy is to consider the classical phase space of the FLRW model coupled to matter, but now equipped with the quantum-corrected Hamiltonian constraint. This constraint and the Hamilton's equations of motion it determines provide the full set of effective Einstein's equation for the FLRW model.

In order to obtain the modified Friedmann equation, one first computes the Hamilton's equation for ν:

$$\dot{\nu} = \{\nu, C_H^{(\text{eff})}\} = -\frac{2}{\hbar}\frac{\partial}{\partial b}C_H^{(\text{eff})} = \frac{3}{\gamma\lambda}\nu \sin(\lambda b)\cos(\lambda b). \tag{5.4}$$

Next, since physical solutions also satisfy the constraint $C_H^{(\text{eff})} \approx 0$, we also have

$$\frac{3\hbar}{4\gamma\lambda^2}\nu \sin^2(\lambda b) = \mathcal{H}_{\text{matt}}. \tag{5.5}$$

On using relation (2.41) between ν and the physical volume, this equation can be rewritten as

$$\frac{\sin^2(\lambda b)}{\gamma^2\lambda^2} = \frac{8\pi G}{3}\rho, \tag{5.6}$$

where, as before, ρ is the energy density of matter. Squaring (5.4) and using (5.6), we obtain

$$H^2 = \frac{\dot{v}^2}{9v^2} = \frac{8\pi G}{3}\rho\left(1 - \frac{\rho}{\rho_{\max}}\right), \tag{5.7}$$

where $H = \dot{a}/a$ denotes the Hubble rate and $\rho_{\max}$ is the maximum energy density given by $\rho_{\max} = 3/(8\pi G\gamma^2\lambda^2) \approx 0.41\rho_{\text{Pl}}$. This is the modified Friedmann equation we were seeking. Note that in the expression of the effective constraint (5.6), it is the left-hand side that is modified from b^2 to $\sin^2\lambda b/\lambda^2$ due to the underlying quantum geometry. To arrive at the modified Friedmann equation, we have merely used the equation of motion for v and trignometric identities to shift this modification to the right-hand side.

Similarly, the modified Raychaudhuri equation can be obtained from Hamilton's equation for b:

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\rho\left(1 - 4\frac{\rho}{\rho_{\max}}\right) - 4\pi G P\left(1 - 2\frac{\rho}{\rho_{\max}}\right). \tag{5.8}$$

It is also useful to obtain the equation for the rate of change of the Hubble parameter using the modified Friedmann and Raychaudhuri equations:

$$\dot{H} = -4\pi G(\rho + P)\left(1 - 2\frac{\rho}{\rho_{\max}}\right). \tag{5.9}$$

These equations immediately provide a conservation law of matter,

$$\dot{\rho} + 3H\left(\rho + P\right) = 0. \tag{5.10}$$

Note that although the effective Friedmann and Raychaudhuri equations are modified due to quantum corrections, the conservation law is the same as in classical cosmology. Furthermore, as in the classical theory, equations (5.7), (5.8) and (5.10) form an over-complete set: one can alternatively derive (5.10) from Hamilton's equations for the matter field and then use (5.7) to derive the modified Raychaudhuri equation (5.8).

In general relativity, the field equations lead to a singularity for all matter satisfying the weak energy condition (WEC), except for the special case of a cosmological constant. By contrast, one can show that the modified field equations lead to a non-singular evolution. In particular, equation (5.7) implies that $\dot{a}$ vanishes at $\rho = \rho_{\max}$ and the universe bounces. In the limit $G\hbar \to 0$ or equivalently $\lambda \to 0$, as one would expect, the modified Friedmann and Raychaudhuri equations directly reduce the classical equations:

$$H^2 = \frac{8\pi G}{3}\rho, \qquad \frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3P), \qquad \dot{H} = -4\pi G(\rho + P). \tag{5.11}$$

In this limit, $\rho_{\max}$ also becomes infinite, the bounce disappears and the classical singularity reappears.

Let us now consider the time evolution of the Hubble rate. An interesting phase in the cosmological evolution occurs when $\dot{H} > 0$. This is known as the phase of *super-inflation*, as the acceleration of the universe in this phase is faster than in a de Sitter spacetime. In the classical theory, for all matter satisfying the WEC, $\dot{H}$ is negative. In order to have a super-inflationary phase in general relativity, one needs to violate WEC, e.g., by introducing a phantom matter in the theory (see, for example, [175]). On the other hand, in LQC, the phase of super-inflation is generic: since the universe is in a contracting phase ($H < 0$) immediately before the bounce and since it enters an expanding phase ($H > 0$) immediately after the bounce, it follows that $\dot{H} > 0$ at the bounce and hence, by continuity, also for some time after the bounce. From equation (5.9) one finds that it occurs when $\rho_{\max}/2 < \rho \leqslant \rho_{\max}$, for all matter satisfying the WEC[19]. Initially there was some hope that this phase may provide

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[19] Interestingly, if one considers matter which violates the WEC, then it does not lead to super-inflation in LQC when $\rho_{\max}/2 < \rho \leqslant \rho_{\max}$ [172].

the accelerated expansion invoked in the inflationary scenarios without having to introduce an inflaton with a suitable potential [40]. However, in general, the phase is extremely short lived and therefore cannot be a substitute of the standard slow roll. But it has interesting phenomenological ramifications, e.g., for the production of primordial gravitational waves.

Remarks.

(1) Note that the full set of effective equations has two key properties: (i) they are free from infrared problems because they reduce to the corresponding equations of general relativity when $\rho \ll \rho_{max}$ and (ii) they are all independent of the initial choice of the fiducial cell. Even though they may seem simple and obvious, these viability criteria are not met automatically [176] but require due care in arriving at effective equations.

(2) The possibility of a phase of super-inflation in LQC was first noted using a different mechanism than the one discussed here [40]. Inverse volume effects can provide additional corrections to the modified Friedmann equations which result in $\dot{H} > 0$. These were first noted for a scalar field in [40] and were subsequently generalized to matter satisfying $P = P(\rho)$ [177]. With these corrections, the conservation law (5.10) also gets modified by additional terms and the effective equation of state of matter changes [177]. If one assumes an effective Hamiltonian constraint incorporating purely inverse volume corrections (and neglects all other modifications originating from quantum geometry), super-inflation occurs when the effective equation of state is such that the WEC is violated. Thus, the super-inflationary regime originating from inverse volume corrections is qualitatively different from the one discussed above. Also, these corrections are physical only in the spatially compact case.

5.2.2. The absence of strong curvature singularities. Let us now discuss additional properties of the Hubble rate and curvature invariants in LQC. In the classical theory of the $k = 0$, $\Lambda = 0$ FLRW models, the Hubble rate diverges for all matter satisfying WEC when the scale factor vanishes. By contrast, the Hubble rate in LQC has a universal upper bound. From equation (5.7), it follows that its maximum allowed value occurs at $\rho = \rho_{max}/2$ and is equal to

$$|H|_{max} = \left(\frac{1}{\sqrt{3} 16 \pi G \hbar \gamma^3} \right)^{1/2} \approx 0.93 m_{Pl}. \tag{5.12}$$

It then immediately follows that the expansion of the congruences of cosmological observers is bounded in LQC.

In the homogeneous and isotropic model, Ricci scalar, R, is sufficient to capture the behavior of all other spacetime curvature invariants. For the modified Friedmann dynamics of LQC, the Ricci scalar turns out to be

$$R = 6 \left(H^2 + \frac{\ddot{a}}{a} \right) = 8 \pi G \rho \left(1 + \frac{2\rho}{\rho_{max}} \right) - 24 \pi G P \left(1 - \frac{2\rho}{\rho_{max}} \right). \tag{5.13}$$

Note that unlike the Hubble rate, R depends both on the energy density and pressure of the matter. This opens the possibility that there may exist events where the spacetime curvature may diverge, even though $\rho \leqslant \rho_{max}$. However, such a divergence occurs for a very exotic choice of matter with an equation of state: $P(\rho) \to \pm\infty$, at a finite value of ρ. Interestingly, it can be shown that it is possible to always extend geodesics across such events using modified Friedmann equations [173]. Thus, unlike in general relativity, even if we allow exotic matter, events where spacetime curvature diverges in LQC are not the boundaries of spacetime.

Let us now examine such events in some detail. From the analysis of integrals of curvature components for null and particle geodesics, it is possible to classify the singularities as *strong*

curvature and *weak curvature* types. According to Krölak [178], a singularity occurring at the value of affine parameter $\tau = \tau_e$ is strong if and only if

$$\int_0^\tau d\tau \, R_{ab} u^a u^b \to \infty \qquad \text{as} \quad \tau \to \tau_e. \tag{5.14}$$

Otherwise the singularity is weak. One can show that this integral is finite in the isotropic and homogeneous LQC, *irrespective of the choice of the equations of state* including the ones which lead to a divergence in the Ricci scalar [173]. Thus, the events where spacetime curvature blows up in LQC are harmless weak singularities.

The finiteness of the integral (5.14) can also be used to show that there exist no strong curvature singularities in LQC[20]. This result is in sharp contrast to the situation in general relativity where strong curvature singularities are generic features of the theory.

The generic resolution of strong curvature singularities using the modified Friedmann dynamics implies that not only the big bang and the big crunch, but singularities such as the big rip studied in various phenomenological models are also resolved due to underlying quantum geometric effects [173, 179]. By contrast, such singularities are difficult to avoid in general relativity unless the parameters potential of the phantom field are appropriately fine tuned [175]. However, singularities such as the sudden singularities, which occur due to divergence in pressure with energy density remaining finite, will not be resolved [173, 180]. It turns out that such singularities are always of the weak curvature type, which are harmless and beyond which geodesics can be extended [173]. It is rather remarkable that quantum geometric effects in LQC are able to distinguish between harmful and harmless singularities, and resolve all those which are harmful.

Remark. Strong and weak singularities have also been analyzed in the presence of spatial curvature using modified Friedmann dynamics in LQC, including the cases where they occur in the past evolution [174]. Using a general phenomenological model of the equation of state, one finds that all strong curvature singularities in $k = 1$ and $k = -1$ models are resolved. Furthermore, for the spatially closed model, there exist some cases where even weak curvature singularities may be resolved. This brings out the non-trivial role played by the intrinsic curvature which enriches the new physics at the Planck scale in LQC.

5.3. Probability for inflation in LQC

The inflationary paradigm has been extremely successful in accounting for the observed inhomogeneities in the CMB which serve as seeds for the subsequent formation of the large scale structure in the universe. Consequently, it is widely regarded as the leading candidate to describe the very early universe. However, it faces two conceptual issues. First, as we discussed in section 4.3, Borde, Guth and Vilenkin [159] have shown that the inflationary spacetimes are necessarily past incomplete; even with eternal inflation one cannot avoid the initial big bang. In LQC, on the other hand, thanks to the quantum geometry effects, the singularity is resolved and inflationary spacetimes are past complete.

The second issue is that of 'naturalness'. While a given theory—such as general relativity—may admit solutions with an appropriate inflationary phase, is the occurrence of such a phase generic, or, does it require a careful fine tuning? For definiteness, let us suppose we have an inflaton ϕ with a quadratic potential, $V(\phi) = (1/2)m^2\phi^2$. Then, the WMAP data [157] provides us with a remarkably detailed picture of the conditions at the onset of inflation [83]. More precisely, the data refer to the time $t(k_\star)$ at which a reference

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[20] The classification of the strength of singularities is slightly different in Tipler's analysis [178]. One can show that strong curvature singularities are absent in LQC also using Tipler's criteria.

mode $k_\star$ used by WMAP exited the Hubble horizon in the early universe. (Today, this mode has a wavelength of about 12% of the radius of the Hubble horizon.) Within error bars of less than 4.5%, the data show us that the field configurations were

$$\phi(t(k_\star)) = \pm 3.15 \, m_{\mathrm{Pl}}, \qquad \dot{\phi}(t(k_\star)) = \mp 1.98 \times 10^{-7} m_{\mathrm{Pl}}^2,$$
$$H(t(k_\star)) = 7.83 \times 10^{-6} m_{\mathrm{Pl}}, \tag{5.15}$$

where, as before, $H = \dot{a}/a$ is the Hubble parameter [83]. Thus, for the quadratic potential, the 7 year WMAP data require the dynamical trajectory of the universe to have entered a *tiny* neighborhood of the phase-space point given by (5.15). One's first reaction would be that this condition would be met only by a *very* small fraction of all dynamical trajectories. If so, *a priori* the required inflationary phase would seem very implausible and the theory would be left with a heavy burden of 'explaining' why it actually occurred.

Issue of 'naturalness' has, of necessity, a subjective element and one could just say that our universe simply happened to pass through this tiny region of phase space and, since we have only one universe, the issue of likelihood is irrelevant. However, the broader community did not adopt this viewpoint. Rather, it has sought to sharpen the question of naturalness by introducing a measure on the space $\mathbb{S}$ of solutions of the given theory: the required probability is then given by the *fractional* volume occupied by those solutions which do pass through configurations specified by the WMAP data at some time during their evolution.

To find the measure, the following general strategy was introduced over 20 years ago [181–183]. Recall that solutions to the field equations are in 1–1 correspondence with phase space trajectories, and the natural Liouville measure $d\mu_L$ on the phase space is preserved by the dynamical evolution. On the one hand, this measure is natural because it is constructed using *just* the phase space structure. On the other hand, precisely for the same reason, it does not encode additional information that may be important for the physics of the specific system. Therefore, it only provides *a priori* probabilities, i.e. 'bare' estimates. Further, physical input can and should be used to provide sharper probability estimates and a more reliable likelihood. However, *a priori* probabilities themselves can be directly useful if they are very low or very high. In these cases, it would be an especially heavy burden on the fundamental theory to come up with the physical input that significantly alters them.

The question of probability of inflation along these lines has received a considerable attention in the literature (see, e.g., [184–188]). In the general relativity literature, conclusions on the probability of inflation have been vastly different, ranging from near unity [184] to being exponentially suppressed [185] (by factors of $\sim e^{-195}$ for the slow roll phase associated with configurations (5.15)). It turns out that these vast differences arise because procedure is intrinsically ambiguous within general relativity and different calculations in fact answer different questions. This is a rather subtle issue and, although it is explained in detail in [83, 84], it is still sometimes overlooked (see, e.g., [189]).

Let us discuss this point in some detail in the $k = 0$ FLRW model with a scalar field in a potential $V(\phi)$ (which is bounded below) either in general relativity or in effective LQC. Let Γ denote the four-dimensional phase space, spanned by $(v, b; \phi, p_{(\phi)})$. (Recall that v is related to the scale factor via $v \sim a^3$ and that, in general relativity, $b \sim H$, the Hubble parameter.) Let $\bar{\Gamma}$ denote the constraint surface which can be coordinatized by (v, b, ϕ) and let $\hat{\Gamma}$ be the two-dimensional (gauge-fixed) sub-manifold of $\bar{\Gamma}$ such that each dynamical trajectory intersects it once and only once. Since b is monotonic both in general relativity and LQC, one typically chooses $\hat{\Gamma}$ to be the sub-manifold of $\bar{\Gamma}$ with $b = b_o$, a constant, so that $\hat{\Gamma}$ is coordinatized simply by (v, ϕ). The space $\mathbb{S}$ of solutions is naturally isomorphic with $\hat{\Gamma}$. The pullback $\hat{\Omega}$ to $\hat{\Gamma}$ of the symplectic structure Ω on Γ then provides the natural Liouville measure $d\hat{\mu}_L$

on $\hat{\Gamma}$ and therefore on $\mathbb{S}$. Because the measure is preserved under dynamical evolution, it is insensitive to the choice of gauge fixing, i.e. the value of b_o.

The problem however is that the total Liouville measure of $\mathbb{S}$ is *infinite* and the volume of the subset of $\mathbb{S}$ spanned by solutions which enter the phase space region singled out by the WMAP data is also *infinite*. Therefore, calculations of probabilities can give any answer one pleases. However, the infinities are spurious. For, there is a gauge group $\mathbb{G}$ that acts on the solution space, $v(t) \rightarrow \alpha v(t)$, $\phi(t) \rightarrow \phi(t)$ under which physics does not change. (In terms of scale factors, the action is just $a(t) \rightarrow \beta a(t)$, $\phi(t) \rightarrow \phi(t)$, with $\alpha = \beta^3$.) The infinity in the Liouville volume arises simply from the fact that the 'length' of this gauge orbit is infinite. Therefore, one would like to factor out by this gauge group and be left with a one-dimensional space, spanned by ϕ, with finite total measure. The problem is that although the group $\mathbb{G}$ does have a well-defined action on the space $\mathbb{S}$ of solutions, the symplectic structure $\hat{\Omega}$ and hence the Liouville measure $\mathrm{d}\hat{\mu}_\mathrm{L}$ *fail to be invariant* under the action of $\mathbb{G}$ [83]. So we cannot unambiguously project $\mathrm{d}\hat{\mu}_\mathrm{L}$ down to the space of orbits of $\mathbb{G}$! Rather than projection, one can simply do a second gauge fixing, i.e. choose a cross-section $\tilde{\mathbb{S}}$ of $\mathbb{S}$ (or, equivalently, of $\hat{\Gamma}$) which is traversed by the orbits of $\mathbb{G}$ once and only once. Then, one can *unambiguously* define a measure $\mathrm{d}\tilde{\mu}_\mathrm{L}$ on $\tilde{\mathbb{S}}$ (up to an irrelevant overall constant). In effective LQC, one obtains [82, 83]

$$\mathrm{d}\tilde{\mu}_\mathrm{L} = \left(\frac{3\pi}{\lambda^2} \sin^2 \lambda b_o - 8\pi^2 \gamma^2 V(\phi) \right)^{\frac{1}{2}} \mathrm{d}\phi, \tag{5.16}$$

and the answer in general relativity is given by taking the limit $\lambda \rightarrow 0$ that sends the area gap to zero. The total measure of $\tilde{\mathbb{S}}$ is *finite* in both theories because the matter energy density is fixed on the surface $b = b_o$, whence ϕ ranges over a finite closed interval. As a result, calculations of probabilities yield well defined, finite results. However, the subtlety is that the measure $\mathrm{d}\tilde{\mu}_\mathrm{L}$ *depends on the initial choice* $b = b_o$ *we made to arrive at* $\hat{\Gamma}$ in a non-trivial fashion!

To summarize, the Liouville measure $\mathrm{d}\hat{\mu}_\mathrm{L}$ on the space $\mathbb{S}$ of solutions is unambiguous, independent of the gauge fixing choice $b = b_o$. But the total Liouville volume of $\mathbb{S}$ is infinite. Since this infinity can be directly traced back to the freedom in rescaling $a(t)$ under which physics does not change, it is natural to get rid of the spurious infinity by gauge fixing. This procedure does lead us to a natural measure $\mathrm{d}\tilde{\mu}_\mathrm{L}$ on the space $\tilde{\mathbb{S}}$ of *physically distinct* solutions. But this measure now carries a memory of the choice of b_o, which, in the spacetime picture, corresponds to a choice of a time slice in the solution.

In LQC, we are interested in the evolution to the future of the bounce and the specification of ϕ at the bounce surface suffices to determine a unique *physical* solution in $\tilde{\mathbb{S}}$. The measure $\mathrm{d}\tilde{\mu}_\mathrm{L}$ enables us to ask and answer the following question: What is the *fractional* volume occupied by the subset of all possible $\{\phi\}_\mathrm{B}$ at the bounce surface whose evolution is compatible with the stringent requirements of WMAP? This fraction is the *a priori* probability for initial data at the bounce to lead to a slow roll inflation compatible with the WMAP data some time in the future.

To carry out the calculation, one has to fix the potential. For the quadratic potential, $V(\phi) = (1/2)m^2\phi^2$, the issue was analyzed in detail in [83]. The answer turned out to be *extremely* close to 1: the probability that the dynamical trajectory does *not* pass through the desired configuration (5.15) within the WMAP error bars is *less than* 3×10^{-6}! Let us amplify this statement. The allowed range of ϕ values at the bounce is $|\phi_\mathrm{B}| \leqslant 7.44 \times 10^5 m_\mathrm{Pl}$ and *all* trajectories that start out with $|\phi_\mathrm{B}| > 5.46 m_\mathrm{Pl}$ pass through the tiny phase space region selected by WMAP sometime to the future of the bounce. Note that the matter density at the bounce is $\rho \approx 0.41 \rho_\mathrm{Pl}$, while that at the 'onset of the WMAP slow roll' (i.e. corresponding to

configuration (5.15)) is $\rho \approx 7.32 \times 10^{-12} \rho_{\mathrm{Pl}}$. Therefore, at the 'onset', the allowed range of ϕ is $|\phi_{\mathrm{onset}}| \leqslant 3.19 m_{\mathrm{Pl}}$ and the WMAP allowed region fills only 4.4% of the full allowed range. Thus, trajectories from all but a $\sim$ millionth part of the allowed values of ϕ at the bounce flow to a small region of the allowed values of ϕ at the onset of inflation. In this precise sense, the small region selected by WMAP is an attractor for the effective LQC dynamics [84, 190]. The details of the effective LQC dynamics across these 11 orders of magnitude in density and curvature have a rich structure [83]. It is quite non-trivial that this attractor behavior is realized in spite of the fact that the LQC dynamics is rather intricate and exhibits qualitative differences from general relativity: for example, certain scaling relations are now violated and there is a novel super-inflation phase.

In general relativity, the natural substitute for the big bounce—i.e. the natural time to specify initial conditions—is the big bang. But because of the classical singularity, we cannot carry out this calculation of the *a priori* probability there. And there is no other natural instant of time. One might think of specifying the initial ϕ at the Planck density [184] and use the Liouville measure $\mathrm{d}\tilde{\mu}_{\mathrm{L}}$ attuned to that time. But there is no reason to believe that we can trust general relativity in that era. Alternatively, one can wait till we are in an era where we can trust general relativity [185]. But the answer will depend sensitively on one's choice of b_o used to carry out the calculation because there is simply no natural time instant in this regime. Probabilities calculated in this manner refer to the fractional volume occupied by the initial data *at that rather arbitrary time* which is compatible with the WMAP slow roll. As our discussion above illustrates, later the time, lower will be the probability.

Let us summarize. In the literature, one often asks for the probability that there are a specified number N of e-foldings. In general relativity, this question is rather loose because one does not specify when one should start counting and if one begins at the big bang, the number would be infinite. We asked a sharper question: given a quadratic potential, what is the *a priori* probability of obtaining slow roll inflation that is compatible with the 7 year WMAP data? But even this question is ambiguous because of the subtleties associated with the Liouville measure. One has to fix a time instant, consider all allowed field configurations at that time, and ask for the fractional $\mathrm{d}\tilde{\mu}_{\mathrm{L}}$-volume of the subset of these configurations which, upon evolution, enter the small region of phase space singled out by WMAP. In LQC, there is a natural choice of the initial time—the bounce time—and the detailed investigation then shows that these initial field configurations will meet the desired WMAP region some time in the future with probability that is greater than $(1 - 3 \times 10^{-6})$. In this precise sense, *assuming an inflation in a suitable potential*, an inflationary phase compatible with the WMAP data is almost inevitable in LQC. In general relativity, because there is no natural 'time' for one to specify initial configurations, and because the probability depends on one's choice, answers become less interesting.

5.4. Effective dynamics of Bianchi I spacetimes

As in the case of isotropic models, one can write an effective Hamiltonian constraint in the Bianchi models to capture the underlying quantum dynamics and use it to derive modified dynamical equations incorporating non-perturbative quantum gravity effects. We will again find that there are striking differences from classical general relativity; in particular, the energy density and the shear scalar are bounded in effective LQC. We will conclude this subsection with an application of this modified Bianchi I dynamics to one of the problems faced by the cyclic/ekpyrotic model.

5.4.1. Modified dynamical equations. The effective Hamiltonian for the Bianchi I spacetime can be written as

$$C_H^{(I,\text{eff})} = -\frac{1}{8\pi G \gamma^2 (p_1 p_2 p_3)^{1/2}} \left(\frac{\sin(\bar{\mu}_1 c_1)}{\bar{\mu}_1} \frac{\sin(\bar{\mu}_2 c_2)}{\bar{\mu}_2} p_1 p_2 + \text{cyclic terms} \right) + \mathcal{H}_{\text{matt}}, \quad (5.17)$$

where $\bar{\mu}_i$ are given by equation (4.31). Using Hamilton's equations, one can calculate the time variation of triads and connections and show that $(p_i c_i - p_j c_j)$ is a constant of motion (where, as before, there is no summation over repeated covariant indices). However, unlike in general relativity, the modified dynamical equations now imply that Σ^2 of equation (4.30) is not a constant of motion [163].

Next, let us consider the matter density ρ and the shear scalar $\sigma^2 = 6\Sigma^2/a^6$. The density is now given by

$$\rho = \frac{1}{8\pi G \gamma^2 \lambda^2} \left(\sin(\bar{\mu}_1 c_1) \sin(\bar{\mu}_2 c_2) + \text{cyclic terms} \right), \quad (5.18)$$

whence it is clear that it has an absolute maximum, given by

$$\rho_{\text{max}} = \frac{3}{8\pi G \gamma^2 \lambda^2}. \quad (5.19)$$

Note that the maximum is identical to the upper bound on the energy density in the isotropic model. The expression for σ^2 can be computed by finding the equations for the directional Hubble rates $H_i = \dot{a}_i/a_i$, which after some computation yields

$$\sigma^2 = \frac{1}{3\gamma^2\lambda^2}[(\cos(\bar{\mu}_3 c_3)(\sin(\bar{\mu}_1 c_1) + \sin(\bar{\mu}_2 c_2)) - \cos(\bar{\mu}_2 c_2)(\sin(\bar{\mu}_1 c_1) + \sin(\bar{\mu}_3 c_3)))^2$$

$$+ (\cos(\bar{\mu}_3 c_3)(\sin(\bar{\mu}_1 c_1) + \sin(\bar{\mu}_2 c_2)) - \cos(\bar{\mu}_1 c_1)(\sin(\bar{\mu}_2 c_2) + \sin(\bar{\mu}_3 c_3)))^2$$

$$+ (\cos(\bar{\mu}_2 c_2)(\sin(\bar{\mu}_1 c_1) + \sin(\bar{\mu}_3 c_3)) - \cos(\bar{\mu}_1 c_1)(\sin(\bar{\mu}_2 c_2) + \sin(\bar{\mu}_3 c_3)))^2]. \quad (5.20)$$

This expression implies that σ^2 has the maximum value [191]:

$$\sigma^2_{\text{max}} = \frac{10.125}{3\gamma^2\lambda^2}. \quad (5.21)$$

These bounds bring out a key difference between the isotropic and anisotropic cases. In the isotropic case, there is a single curvature scalar and it—as well as the energy density—assumes the maximum value at *the* bounce. In the anisotropic case, by contrast, the Weyl curvature is non-zero and shears serve as its (gauge invariant) potentials. Since both the density and shears have an upper bound, one now has not just one bounce where the density assumes its maximum value, but other 'bounces' as well, associated with shears. There are regimes in which the shear grows and assumes its upper limit. At that time, the energy density is not necessarily maximum. Still the quantum geometry effects grow enormously, overwhelm the classical growth of shear, diluting it, and avoid the singularity. Thus, the effective dynamics leads to the following qualitative picture: any time a curvature scalar enters the Planck regime, the 'repulsive' forces due to quantum geometry effects grow and cause a bounce in that scalar. Thus, even in the homogeneous case, the bounce structure becomes much more intricate and physically interesting.

The complicated form of the modified dynamical equations in the Bianchi I model makes the task of writing an analog of the generalized version of Friedmann-like equation (4.29), very difficult in LQC. However, if we neglect terms of the order $(\bar{\mu}_i c_i)^4$ and higher, then one can derive such an equation by following the steps as outlined in the isotropic case, and it turns out to be [163]

$$H^2 = \frac{8\pi G}{3}\rho\left(1 - \frac{\rho}{\rho_{\text{max}}}\right) + \frac{\Sigma^2_{\text{cl}}}{a^6}\left(1 - 3\frac{\rho}{\rho_{\text{max}}}\right) - \frac{9}{8\pi G}\frac{\Sigma^4_{\text{cl}}}{\rho_{\text{max}}a^4} + O((\bar{\mu}_i c_i)^4). \quad (5.22)$$

Here, Σ_{cl} the value of Σ in the classical limit of the theory. Unfortunately, this equation only captures the dynamics faithfully only when anisotropies are small. It will be interesting to obtain the generalized Friedmann and Raychaudhuri equations using the effective Hamiltonian constraint without such approximations.

5.4.2. Singularity resolution in the ekpyrotic/cyclic model. An interesting application of the effective LQC dynamics is to the ekpyrotic/cyclic model. In this paradigm, one makes the hypothesis that the universe undergoes cycles of expansion and contraction driven by a scalar field in a potential of the form [192]

$$V(\phi) = V_c \left(1 - \mathrm{e}^{-\sigma_1 \phi}\right) \exp(-\mathrm{e}^{-\sigma_2 \phi}), \tag{5.23}$$

where V_c, σ_1 and σ_2 are the parameters of the model. The model has been proposed as an alternative to inflation, where the contracting branch plays an important role in the generation of structures in the universe.

Various stages of the evolution can be summarized as follows. In the contracting phase, the field ϕ evolves from the positive part of the potential and enters the steep negative well where its equation of state becomes ultrastiff. This phase of evolution is thought to be responsible for the generation of nearly scale invariant perturbations in the universe. After passing through the steep negative region of the potential, the field rolls toward $\phi = -\infty$ which corresponds to the big-crunch singularity. If one can somehow continue the evolution through this big crunch and if the field rolls back in the expanding branch from $\phi = -\infty$, then at late times it can lead to an accelerated expansion of the universe. Eventually, the expansion of the universe stops due to Hubble friction and the universe enters into a contracting phase to repeat the cycle.

Note that the model faces a dual challenge: one has to obtain a non-singular transition of the scale factor of the universe, and furthermore, one has to achieve a turnaround of ϕ in the vicinity of $\phi = -\infty$. It is relatively straightforward to see from the classical Friedmann equation that such a turnaround is not possible when the potential is negative. In any case, the classical dynamical equations are inadequate to address these key issues because they cannot be trusted in the regime near the singularity. A natural question then is whether non-perturbative quantum gravity effects encoded in dynamical equations in LQC can provide insights on the singularity resolution in the ekpyrotic/cyclic model and, if so, whether the scalar field undergoes the desired turnaround in the ensuing dynamics. This issue has been analyzed both in the isotropic and anisotropic versions of the model. In the isotropic case, one finds that as the scalar field rolls toward $\phi = -\infty$, its energy density rises and approaches $\rho_{\max}$. Once it equals $\rho_{\max}$, the scale factor of the universe bounces and the singularity is avoided [190].[21] However, the scalar field does not turn around and it continues rolling toward $\phi = -\infty$. By contrast, if one considers the effective dynamics of the Bianchi I model, one finds that not only is the singularity resolved but also the field turns around for a large range of initial conditions [194]. The turnaround of the field is tied to the non-trivial role played by the shear scalar in the dynamical equations, and occurs even if the anisotropies are small.

In figure 7, we show the results from a numerical analysis of the effective dynamical equations with the ekpyrotic/cyclic potential. It depicts a rich structure of multiple bounces in the Planck regime, and a turnaround of ϕ leading to a viable cycle. Figure 8 shows the behavior of the energy density and the shear scalar. Since the anisotropies are non-vanishing, the energy density does not reach its maximum value $\rho_{\max}$ when the scale factor bounces in

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[21] The singularity resolution in the ekpyrotic/cyclic model was first considered in the isotropic LQC in [193]. However, modifications to the effective dynamics originating from the non-local nature of the field strength tensor were ignored in that work.
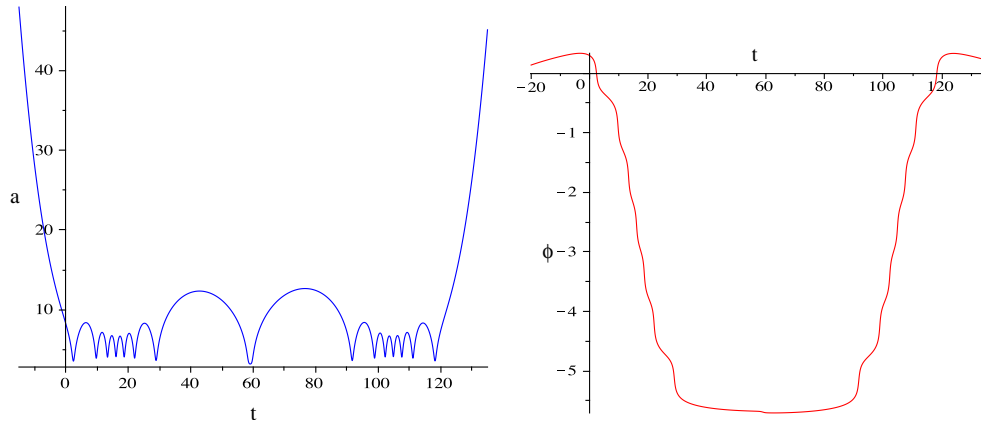
Figure 7. Plot of the behavior of the scale factor and the scalar field in effective loop quantum dynamics of Bianchi I with potential (5.23). The choice of the parameters are $V_c = 0.01$, $\sigma_1 = 0.3\sqrt{8\pi}$ and $\sigma_2 = 0.09\sqrt{8\pi}$. The initial values are $\phi = 0.4$, $\dot{\phi} = -0.03$, $p_1 = 64$, $p_2 = 72$, $p_3 = 68$, $c_1 = -0.6$ and $c_2 = -0.5$. (All units are Planckian.) The initial value of c_3 was determined using the vanishing of the Hamiltonian constraint.
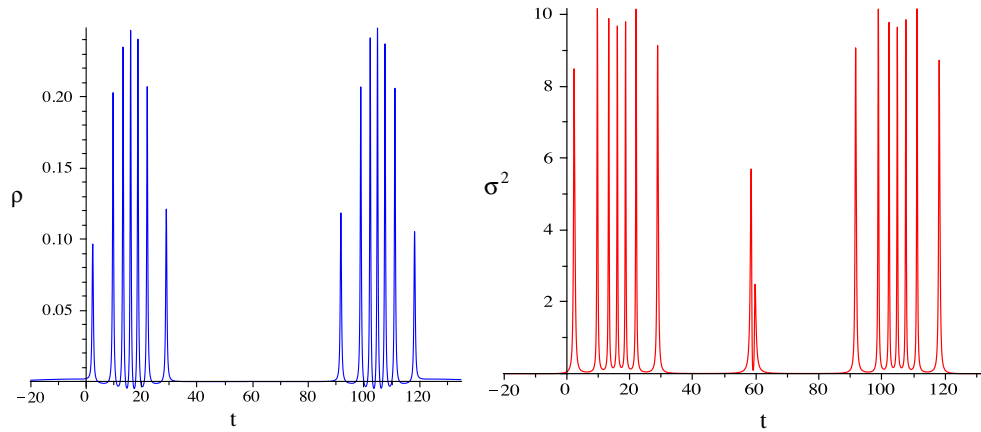

Figure 8. Behavior of the energy density and the shear scalar σ^2. Parameters in this plot are the same as those in figure 7. The plot of energy density shows slight negative values, which occur when the potential is negative. The Hubble rate remains real, and the evolution is well defined in this regime because of the compensation from the shear scalar term, which is always positive.

the Planck regime. For a deeper understanding of the viability of this model, further work is needed to quantify the constraints on the required magnitude of anisotropies. However, current studies show that they can be very small [194]. Thus, modified dynamics of the Bianchi I model in LQC successfully resolves a challenging problem of the ekpyrotic/cyclic model. Note that attempts to resolve this problem using ghost condensates, such as in the 'new ekpyrotic scenario' [195], encounter problems of instabilities [196]. In contrast, in effective LQC, one does not need to introduce exotic matter to resolve the singularity, and there are no such instability problems.

5.5. Summary of other applications

Pre-big-bang models and LQC. The proposal of pre-big-bang models [18], based on string cosmology, is an attractive idea but faces the problem of non-singular evolution from the contracting to the expanding branch. A phenomenological study based on exporting the non-perturbative quantum gravitational effects as understood in LQC to these models reveals that this problem can be successfully resolved both in the Einstein and the Jordan frame without any fine tuning of the initial conditions [197]. Similar results have been derived in the presence of a positive potential [198]. Thus, modified FLRW dynamics in LQC alleviates a major problem of the pre-big-bang scenarios and provides a clear insight in the form of the required non-perturbative terms from higher order effective actions in the string cosmologies.

Covariant action for LQC. A natural question in LQC is whether the modified Friedmann dynamics can be obtained from a covariant effective action. The issue is subtle because while isotropic LQC has only two gravitational degrees of freedom, effective actions in the conventional treatments generally require additional degrees of freedom. Furthermore, for metric theories, the requirements of second-order dynamical equations and covariance uniquely lead to the Einstein–Hilbert action up to a cosmological constant term. However, if one generalizes to theories where the metric and the connection are regarded as independent, one *can* construct a covariant effective action that reproduces the effective LQC dynamics [199].[22] For a simple functional form, $f(\mathcal{R})$ where $\mathcal{R}$ is the curvature of the independent connection, the action turns out to be an infinite series in $\mathcal{R}$. It is possible that the functional form of the effective action is not unique and various effective actions involving higher order curvature invariants such as $\mathcal{R}_{\mu\nu}\mathcal{R}^{\mu\nu}$ exist. Nonetheless, the availability of an effective action capturing non-perturbative quantum gravity modifications has sparked considerable interest in the construction of loop-inspired non-singular models in the Palatini theories (see [201] for a review).

Correspondence with braneworld scenarios and scaling solutions. Interestingly, properties of solutions to the modified Friedmann dynamics in LQC have some similarities and dualities with properties of solutions in the braneworld scenarios (see [202] for a comprehensive review of braneworlds). These have been investigated in two ways. First, by considering the modifications to the matter Hamiltonian originating from inverse scale factor effects [203] and second by modifications to the gravitational part of the Hamiltonian constraint [172]. The latter bear a more natural analogy with the braneworld cosmologies where one obtains ρ^2 modifications albeit with an opposite sign. Therefore, in the braneworld scenarios, bounces can occur only if the brane tension is allowed to be negative [204]. Finally, scaling solutions have been obtained in effective LQC both for equations resulting from the modification of the gravitational part of the Hamiltonian constraint [205, 206] and from the modifications in the matter Hamiltonian coming from inverse scale factor effects [207]. These facilitate qualitative comparison of the effective LQC dynamics with that in the braneworld scenarios.

Dark energy models in LQC. Dynamical behavior of various dark energy models have been studied using the modified Friedman equations in LQC and comparisons have been made with general relativity. These include interacting dark energy model with dark matter [208]; multi-fluid interacting model in LQC [209]; dynamics of phantom dark energy model [210];

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[22] Attempts have also been made to write an effective action in a metric theory, but these have not been successful in capturing the regime in which non-perturbative quantum gravitational effects become significant, including the bounce [200].

quintessence and anti-Chaplygin gas [211] and quintom and hessence models [212]. The latter have also been used to construct non-singular cyclic models [213].

Tachyonic fields. Various applications of tachyonic matter have been studied in LQC. The singularity resolution has shown to be robust [214] and attractors have been found for a tachyon in an exponential potential [215]. The results on tachyonic inflationary scenario have been recently extended to the warm inflation [216] (see also [217] for another warm inflationary model in LQC).

Singularity resolution in the k = 1 model. In section 4.1, we discussed the loop quantization of the $k = 1$ model with a massless scalar field as the source and demonstrated the singularity resolution. Using the effective Hamiltonian constraint, the resolution of singularities has been studied for more general forms of matter. Since the spacetime is spatially compact, inverse volume corrections are well defined and they lead to some interesting features. It can be shown that the scale factor in the $k = 1$ model undergoes bounces even if one includes only the inverse volume modifications to the effective Hamiltonian constraint [218]. For steep potentials, where the initial conditions to resolve the singularity have a set of measure zero in general relativity, bounce occurs in LQC under generic conditions. A generalization has recently been investigated in the Lemaitre–Tolman geometries where again only the inverse volume corrections are included and occurrence of bounces has been compared between marginal and non-marginal cases [219]. In another application [220], bounces have also been studied in an alternative quantization which captures the elements of quantization used in Bianchi II [61] and Bianchi IX models [62] (see section 4.4.2 for details).

Bianchi I models and magnetic fields. An important application of the effective dynamics in Bianchi models deals with the study of matter with a non-vanishing anisotropic stress. Such a matter-energy stress tensor leads to non-conservation of the shear scalar (Σ^2) in the classical theory as well as LQC. It is of interest to understand how the presence of such matter affects the bounce in LQC. By including magnetic fields, an investigation on these lines was carried out in [221]. The result is that the bounds on energy density and shear scalar in the Bianchi I model are not affected, although there is a significant variation in anisotropies across the bounce.

Physics of Bianchi II and Bianchi IX models. Effective Hamiltonian constraints of Bianchi II and Bianchi IX models, obtained in [61] and [62] respectively, have been used to explore some of their physical consequences in detail [191]. It turns out that while one can obtain an upper bound on the energy density ρ without imposing energy conditions in the Bianchi II model, in contrast to the Bianchi I model, these conditions are now necessary to bound the shear scalar σ^2. In the Bianchi IX model, because of the spatially compact topology, inverse volume corrections to the effective Hamiltonian constraint are meaningful and have to be included. They turn out to play an important role in placing an upper bound on the energy density. In both of these models, the upper bounds on the energy density and the shear scalar, obtained by imposition of the WEC, turn out to be higher than the universal bounds in the Bianchi I model: they turn out to be $\rho_{max} \approx 0.54\rho_{Pl}$ and $\sigma^2_{max} \approx 127.03/(3\gamma^2\lambda^2)$ in the Bianchi II model and $\rho \approx 7.91\rho_{Pl}$ and $\sigma^2_{max} \approx 1723.64/(3\gamma^2\lambda^2)$ in the Bianchi IX model. However, it is not known that these bounds are optimal.

6. Beyond homogeneity

While kinematics of full LQG is well established, there is still considerable ambiguity in the definition of the full Hamiltonian constraint. Nonetheless significant progress has been

made in some inhomogeneous contexts by extending the strategy that has been successful in mini-superspaces. These explorations are phenomenologically important since they have the potential to open new avenues to observable consequences of quantum gravity in the early universe. They are also significant from a more theoretical angle since they provide guidance for full LQG.

In this section, we will discuss three directions in which inhomogeneities are being incorporated: (i) the one-polarization Gowdy midi-superspaces which admit gravitational waves with or without a scalar field as the matter source; (ii) inhomogeneous test quantum fields on cosmological quantum geometries; and (iii) cosmological perturbations on FLRW backgrounds. In each case, one begins with the appropriately truncated (but infinite-dimensional) sector of the classical phase space of full general relativity (with matter), and uses suitable gauge fixing to make quantization tractable. The resulting Hamiltonian theories exhibit a clean separation between homogeneous and inhomogeneous modes and, mathematically, one can regard the inhomogeneous modes as an assembly of harmonic oscillators. Quantum theory is then constructed by treating the homogeneous modes in the manner of LQC and the inhomogeneous modes as in the standard Fock theory. It is quite non-trivial that this 'hybrid' procedure provides a coherent, non-perturbative quantization of an infinite-dimensional phase space, consistent with the underlying truncation of the full theory.

The relation between these theories and the eventual, full LQG will become clear only once there is a satisfactory candidate for the full Hamiltonian constraint. Nonetheless, it seems reasonable to hope that these truncated theories will provide good approximations to full dynamics for states in which the 'energy' in the inhomogeneities is sufficiently small even in the Planck era [8]. In this case, the inhomogeneous modes will be affected by the quantum geometry effects—such as the bounces—of the dominant homogeneous modes but they would be too weak for their own quantum geometry effects to be important. These conditions are compatible with some of the mainstream inflationary scenarios. Therefore, this approach may also be useful in phenomenological studies.

6.1. The Gowdy models

In the Gowdy midi-superspaces, the spatial manifold is taken to be $\mathbb{T}^3$ and all spacetimes under consideration have two commuting Killing fields. Thus, inhomogeneities are restricted just to one spatial direction. Thanks to these symmetries, one can introduce a geometrically well-motivated gauge fixing procedure, making the model mathematically tractable. If we further require that the two Killing fields be hypersurface orthogonal—so that the gravitational waves have a single polarization—the model becomes exactly soluble classically. Therefore, over the years, the Gowdy midi-superspace—and especially the one-polarization case—has received considerable attention in the mathematical literature on cosmology. Long before the advent of LQG, there were several attempts to quantize this model (see, e.g., [222]). However, in the resulting quantum theories, the initial, big-bang-type singularity could not be naturally resolved. By contrast, thanks to quantum geometry underlying LQC, the singularity has now been resolved both in the vacuum case and in the case when there is a massless scalar field [4–8]. In what follows, we will focus on the vacuum case which has drawn most attention so far.

Let (θ, σ, δ) be the coordinates on $\mathbb{T}^3$ with ∂_σ and ∂_δ as the two hypersurface orthogonal Killing fields. Then, the phase space variables depend only on the angle θ and one can carry out a Fourier decomposition with respect to it. This provides a decomposition of the phase space, $\Gamma = \Gamma_{\text{hom}} \times \Gamma_{\text{inhom}}$, where the homogeneous sector is spanned by the zero (Fourier)

modes and the (purely) inhomogeneous sector, by the non-zero modes. Using underlying symmetries, the inhomogeneous sector can be fully gauge fixed and one is left with only two *global* constraints, the diffeomorphism constraint (C_θ) and the Hamiltonian constraint (C_H), which Poisson commute.

The homogeneous sector Γ_{hom} can be regarded as the phase space of the vacuum Bianchi I model of section 4.4. However, since the spatial manifold is now $\mathbb{T}^3$, we do not need to introduce a cell and can set $L_i = 2\pi$. Quantization of this sector can be performed as in section 4.4.

The inhomogeneous sector Γ_{inhom} can be coordinatized by creation and annihilation variables, a_m and $a_m^\star$ respectively. The global diffeomorphism constraint only contains the inhomogeneous modes and can be written as

$$C_\theta = \sum_{n=1}^{\infty} n(a_n^\star a_n - a_{-n}^\star a_{-n}) \approx 0. \tag{6.1}$$

The Hamiltonian constraint on the other hand involves all modes:

$$C_H^{\text{Gowdy}} = C_H^{(I)} + 32\pi^2\gamma^2|p_\theta|\,H_o + \frac{(c_\sigma p_\sigma + c_\delta p_\delta)^2}{|p_\theta|}H_{\text{int}} \approx 0, \tag{6.2}$$

where $C_H^{(I)}$ is the Bianchi I Hamiltonian constraint (4.28), H_o is the 'free part' of the Hamiltonian of inhomogeneous modes (which represent gravitational waves) and H_{int} is called the 'interaction part' because it mixes the inhomogeneous modes among themselves. The explicit expressions are

$$C_H^{\text{hom}} = -\frac{1}{8\pi G\gamma^2}(c_\theta p_\theta c_\sigma p_\sigma + c_\theta p_\theta c_\delta p_\delta + c_\sigma p_\sigma c_\sigma p_\sigma)$$

$$H_o = \frac{1}{8\pi G\gamma^2}\sum_{n\neq 0}|n|a_n^\star a_n \quad \text{and} \quad H_{\text{int}} = \frac{1}{8\pi G\gamma^2}\sum_{n\neq 0}\frac{1}{2|n|}(2a_n^\star a_n + a_n a_{-n} + a_n^\star a_{-n}^\star). \tag{6.3}$$

Note that H_o and H_{int} depend only on the homogeneous modes and the coupling between the homogeneous and inhomogeneous modes is made explicit in (6.2).

Quantization of the homogeneous sector follows the procedure outlined in section 4.4. On the inhomogeneous sector, one simply uses the Fock quantization, replacing a_n and $a_n^\star$ by annihilation and creation operators. The kinematical Hilbert space thus consists of a tensor product $\mathcal{H}_{\text{kin}}^{\text{Gowdy}} = \mathcal{H}_{\text{kin}}^{(I)} \otimes \mathcal{F}$ of the kinematic Hilbert space of the Bianchi I model and the Fock space generated by the inhomogeneous modes. The full quantum constraint operator is given by [6]

$$\Theta_{\text{Gowdy}} = \Theta_{(I)} + \frac{1}{8\pi\gamma^2}\left[32\pi^2\gamma^2\widehat{|p_\theta|}\hat{H}_o + \left(\widehat{\frac{1}{|p_\theta|^{1/4}}}\right)^2(\hat{\Theta}_\sigma + \hat{\Theta}_\delta)^2\left(\widehat{\frac{1}{|p_\theta|^{1/4}}}\right)^2\hat{H}_{\text{int}}\right], \tag{6.4}$$

where the inverse powers of $|\hat{p}_\theta|$ are defined using the LQC analog of the Thiemann trick [36, 154]. The Bianchi I operator $\Theta_{(I)}$ in these works uses a slightly different—and a more convenient—factor ordering from that in [3] which we used in section 4.4.

Physical states lie in the kernel of the operators $\hat{C}_\theta$ and Θ_{Gowdy}. The physical scalar product is chosen by demanding that a complete set of observables be self-adjoint. The volume $v = \sqrt{p_\sigma p_\delta p_\theta}$ serves as a local internal time as in the classical theory with respect to which the constraint yields a well-posed 'initial value problem'. (Had we introduced a massless scalar field, it would serve as a global internal time.) One can easily check that, as in the Bianchi models, states localized on configurations with zero volume decouple from the rest. In particular, states which initially vanish on zero volume configurations continue

to do so for all time. Thus, the singularity is again resolved. This resolution is sometimes called 'kinematical' to emphasize that it relies on the properties of the constraint operator Θ_{Gowdy} on the kinematical Hilbert space rather than on a systematic analysis of solutions to the quantum constraint in the Planck regime. This nomenclature can be misleading because it may suggest that one only needs the kinematic set up rather than properties of Θ_{Gowdy} that generates dynamics.

Furthermore, details of dynamics have already been explored using effective equations [5, 8] and they show that the behavior observed in the Bianchi I model—including the bounces—carries over to the Gowdy models. The analysis also provides valuable information on the changes in the amplitudes of gravitational waves in the distant past and distant future, resulting from the bounce. A limitation of this analysis is that the effective equations it uses arise from the quantum constraint given in the older papers [152, 162] which, as we discussed in section 4.4, has some unsatisfactory features. However, an examination of the details of the analysis suggests that the qualitative behavior of the solutions of effective equations derived from the corrected quantum constraint of [3, 6] will be the same [223].

In summary, Gowdy models are midi-superspaces which provide an interesting avenue to incorporate certain simple types of inhomogeneities in LQC. Although one often refers to the Bianchi I geometry created by the homogeneous modes as a 'background', it is important to note that this analysis provides an exact—not perturbative—quantization of the one polarization Gowdy model. However, since the LQG effects created by inhomogeneities are not incorporated, it is expected to be only an approximation to the full LQG treatment of the model, but one that is likely to have a large and useful domain of validity.

6.2. Quantum field theory in cosmological, quantum spacetimes

Singularity resolution in Gowdy models is conceptually important because, thanks to their inhomogeneity, they carry an infinite number of degrees of freedom. However, these models do not capture physically realistic situations because their inhomogeneities are restricted to a single spatial direction. To confront quantum cosmology with observations, we must allow inhomogeneities in all three dimensions. However, an exact treatment of these inhomogeneities is not essential: to account for the temperature fluctuations in the CMB, it has sufficed to consider just the first order perturbations, ignoring their back reaction on geometry. Indeed, much of the highly successful analysis in the inflationary paradigm has been carried out in the framework of quantum theory of *test* fields on a FLRW background. In LQC, on the other hand, to begin with we have a *quantum geometry* rather than a smooth curved background. It is therefore of considerable interest to ask if quantum field theory on cosmological *quantum* geometries naturally emerges in a suitable approximation from the Hamiltonian theory underlying LQG and, if so, what its relation is to quantum field theory on FLRW spacetimes, normally used in cosmology.

A priori, it is far from clear that there can be a systematic relation between the two theories. In quantum field theory on FLRW backgrounds, one typically works with conformal or proper time, makes a heavy use of the causal structure made available by the fixed background spacetime, and discusses dynamics as a unitary evolution in the chosen time variable. If we are given just a quantum geometry sharply peaked at a FLRW background, none of these structures are available. Even in the deparameterized picture, it is a *scalar field* that plays the role of internal time; proper and conformal times are at best operators. Even when the quantum state is sharply peaked on an effective LQC solution, we have only a probability distribution for various spacetime geometries; we do not have a single, well-defined, classical causal structure. Finally, in the Hamiltonian framework underlying full LQG, dynamics is

teased out of the constraint. It turns out that, in spite of these apparently formidable obstacles, the standard quantum field theory on curved spacetimes, as practiced by cosmologists, does arise from a quantum field theory on cosmological quantum geometries [86].

In this section, we will summarize this reduction. As explained in section 6.3.1, the underlying framework is expected to serve as a point of departure for a systematic treatment of cosmological perturbations starting from the big bounce where quantum geometry effects play a prominent role.

6.2.1. Setting the stage. While discussing cosmological perturbations, one often uses Fourier decompositions. Strictly speaking, these operations are well defined only if the fields have certain fall-offs which are physically difficult to justify in the homogeneous cosmological settings. Therefore, to avoid unnecessary detours, in this section we will work with a spatially compact case; the $k = 0$, $\Lambda = 0$ FLRW models on a 3-torus $\mathbb{T}^3$. To make a smooth transition from quantum geometry discussed in sections 2 and 3, we will assume that the FLRW spacetime has a (homogeneous) massless scalar field ϕ as the matter source. In addition, there will be an inhomogeneous, free, *test* quantum scalar field φ with mass m. It is not difficult to extend the framework to include spatial curvature or a cosmological constant in the background and/or more general test fields.

Fix periodic coordinates x^i on $\mathbb{T}^3$ with $x^i \in (0, \ell)$. The FLRW metric is given by

$$g_{ab}\, \mathrm{d}x^a \mathrm{d}x^b = -N_{x_0}^2\, \mathrm{d}x_0^2 + a^2 \big(\mathrm{d}x_1^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2\big), \tag{6.5}$$

where the lapse N_{x_0} depends on the choice of the time coordinate x_0; $N_t = 1$ if x_o is the proper time t; $N_\tau = a^3$ if x_0 is the harmonic time τ. Since the solution to the equation of motion for ϕ is $\phi = (p_{(\phi)}/\ell^3)\, \tau$, if we use ϕ as time the lapse becomes $N_\phi = (\ell^3/p_{(\phi)})a^3$. Since $p_{(\phi)}$ is a constant in any solution, N_τ and N_ϕ are just constant multiples of each other in any one spacetime. However, on the phase space, or in quantum theory, we have to keep track of the fact that $p_{(\phi)}$ is a dynamical variable.

In the cosmological literature, quantum fields on a *given* FLRW background are generally discussed in terms of their Fourier modes:

$$\varphi(\vec{x}, x_0) = \frac{1}{(2\pi)^{3/2}} \sum_{\vec{k} \in \mathcal{L}} \varphi_{\vec{k}}(x_0)\, \mathrm{e}^{\mathrm{i}\vec{k} \cdot \vec{x}} \qquad \text{and} \qquad \pi(\vec{x}, x_0) = \frac{1}{(2\pi)^{3/2}} \sum_{\vec{k} \in \mathcal{L}} \pi_{\vec{k}}(x_0)\, \mathrm{e}^{\mathrm{i}\vec{k} \cdot \vec{x}}, \tag{6.6}$$

where, in our case, $\mathcal{L}$ is the three-dimensional lattice spanned by $(k_1, k_2, k_3) \in ((2\pi/\ell)\, \mathbb{Z})^3$, $\mathbb{Z}$ being the set of integers. One often introduces real variables $q_{\vec{k}}$, $p_{\vec{k}}$ via

$$\varphi_{\vec{k}} = \tfrac{1}{\sqrt{2}}(q_{\vec{k}} + \mathrm{i}q_{-\vec{k}}) \qquad \text{and} \qquad \pi_{\vec{k}} = \tfrac{1}{\sqrt{2}}(p_{\vec{k}} + \mathrm{i}p_{-\vec{k}}). \tag{6.7}$$

In terms of the canonically conjugate pairs $(q_{\pm\vec{k}},\ p_{\pm\vec{k}})$, the Hamiltonian becomes

$$H_\varphi(x_0) = \frac{N_{x_0}(x_0)}{2a^3(x_0)} \sum_{\vec{k} \in \mathcal{L}} p_{\vec{k}}^2 + (\vec{k}^2 a^4(x_0) + m^2 a^6(x_0)) q_{\vec{k}}^2. \tag{6.8}$$

(Some care is needed to ensure one does not over-count the modes; see [86].) Thus, the Hamiltonian for the test field is the same as that for an assembly of harmonic oscillators (with time-dependent masses), one for each $\vec{k} \in \mathcal{L}$.

In cosmology, functional analytic issues such as self-adjointness of $\hat{H}_{x_0}$ are generally ignored because attention is focused on a single or a finite number of modes[23]. The time

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[23] See however some recent developments [224] that address the issue of existence and uniqueness of representations of the canonical commutation relations in which dynamics is unitarily implemented in spatially compact cosmological models.

coordinate x_0 is generally taken to be the conformal time or the proper time t. Thus, in a Schrödinger picture, states are represented by wavefunctions $\Psi(q_{\vec{k}}, x_0)$ and evolve via

$$i\hbar \partial_{x_0} \psi(q_{\vec{k}}, x_0) = \hat{H}_{x_0} \psi(q_{\vec{k}}, x_0) \equiv \frac{N_{x_0}(x_0)}{2a^3(x_0)} \big[p_{\vec{k}}^2 + (\vec{k}^2 a^4(x_0) + m^2 a^6(x_0)) q_{\vec{k}}^2 \big] \psi(q_{\vec{k}}, x_0). \quad (6.9)$$

6.2.2. Quantum fields on FLRW quantum geometries. Let us begin with the phase space formulation of the problem. The phase space consists of three sets of canonically conjugate pairs $(\nu, b; \phi, p_{(\phi)}; q_{\vec{k}}, p_{\vec{k}})$. Because we wish to treat φ as a test scalar field whose back reaction on the homogeneous, isotropic background is to be ignored, only the zero mode of the Hamiltonian constraint is now relevant. Thus, we have to smear the Hamiltonian constraint by a constant lapse and we can ignore the Gauss and the diffeomorphism constraint (see section 6.3 for further discussion). As in section 3, let us work with harmonic time so that the lapse is given by $N_\tau = a^3$. Then, the Hamiltonian constraint becomes

$$C_\tau = \frac{p_{(\phi)}^2}{2\ell^3} - \frac{3}{8\pi G} \frac{b^2 V^2}{\ell^3} + H_{\text{test},\tau}, \quad (6.10)$$

where

$$H_{\text{test},\tau} = \frac{1}{2} \sum_{\vec{k}} p_{\vec{k}}^2 + (\vec{k}^2 a^4 + m^2 a^6) q_{\vec{k}}^2. \quad (6.11)$$

As usual, the physical sector of the quantum theory is obtained by considering states $\Psi(\nu, q_{\vec{k}}, \phi)$ which are annihilated by this constraint operator and using the group averaging technique to endow them with the structure of a Hilbert space. Thus, the physical Hilbert space $\mathcal{H}_{\text{phy}}$ is spanned by solutions to the quantum constraint

$$-i\hbar \, \partial_\phi \, \Psi(\nu, q_{\vec{k}}, \phi) = \big[\hat{H}_o^2 - 2\ell^3 \hat{H}_{\text{test},\tau} \big]^{\frac{1}{2}} \Psi(\nu, q_{\vec{k}}, \phi) =: \hat{H} \Psi(\nu, q_{\vec{k}}, \phi), \quad (6.12)$$

which have a finite norm with respect to the inner product

$$\langle \Psi_1 | \Psi_2 \rangle = \frac{\lambda}{\pi} \sum_{\nu=4n\lambda} \frac{1}{|\nu|} \int_{-\infty}^{\infty} dq_{\vec{k}} \, \bar{\Psi}_1(\nu, q_{\vec{k}}, \phi_0) \Psi_2(\nu, q_{\vec{k}}, \phi_0), \quad (6.13)$$

where the right-hand side is evaluated at *any* fixed instant of internal time ϕ_0. In (6.12), $\hat{H}_o := \hbar\sqrt{\Theta}$ governs the dynamics of the background quantum geometry and $\hat{H}_{\text{test},\tau}$ of the test field. The physical observables of this theory are the Dirac observables of the background geometry—such as the time-dependent density and volume operators $\hat{\rho}|_\phi$ and $\hat{V}|_\phi$—and observables associated with the test field, such as the mode operators $\hat{q}_{\vec{k}}$ and $\hat{p}_{\vec{k}}$. (For the background geometry, we use the same notation as in sections 2 and 3.)

The theory under consideration can be regarded as a truncation of LQG where one allows only the *test* scalar field on FLRW geometries. Dynamics has been teased out of the Hamiltonian constraint via deparametrization. Although we started out with harmonic time, τ, as in sections 2 and 3, in the final picture states and observable evolve with respect to the relational time variable ϕ. Note that since ϕ serves as the source of the homogeneous, isotropic background, conceptually this emergent time is rather different from the proper or conformal time traditionally used in cosmology. In the spacetime picture, we have a quantum metric operator on $\mathcal{H}_{\text{phy}}$,

$$\hat{g}_{ab} dx^a dx^b = -\hat{N}_\phi^2 d\phi^2 + (\hat{V}|_\phi)^{\frac{2}{3}} d\vec{x}^2 \qquad \text{with} \quad \hat{N}_\phi =: \hat{V}|_\phi \hat{H}_o^{-1} :, \quad (6.14)$$

where the double dots denote a suitable factor ordering (which must be chosen because $\hat{V}|_\phi$ does not commute with $\hat{H}_o$). In addition, there is a test quantum field $\hat{\varphi}$ that evolves with respect to the internal time coordinate ϕ on the quantum geometry of $\hat{g}_{ab}$.

6.2.3. Reduction.   Let us begin by noting the salient differences between quantum field theory on a classical FLRW background and quantum field theory on quantum FLRW background. In the first case, the time parameter x_0 knows nothing about the matter source that produces the classical, background FLRW spacetime; quantum states depend only on the test field φ (and x_0); and in the expression of the φ-Hamiltonian, the background geometry appears through the externally specified, x_0-dependent parameter a. In the second case, the source ϕ of the FLRW background serves as the relational time parameter; states depend not only on the test field φ but also on the geometry v (and the internal time ϕ); and in the expression of the φ-Hamiltonian, the background geometry appears through *operators* $\hat{a}^4$ and $\hat{a}^6$ which do *not* have any time dependence. Thus, although dynamics has been expressed in the form of Schrödinger equations in both cases, there are still deep conceptual and mathematical differences between the two theories. Yet, the second theory has been shown [86] to reduce to the first one through a series of approximations. We will conclude by briefly summarizing this three-step procedure.

Step 1. One first uses the fact that φ is to be treated as a test field. Therefore, in expression (6.12) of the full Hamiltonian $\hat{H} = \hat{H}_o + \hat{H}_{\text{test},\tau}$, one can regard $\hat{H}_o$ as the 'main part' and $\hat{H}_{\text{test},\tau}$ as a 'perturbation'. After a systematic regularization, the square root in (6.12) can be approximated as

$$[\hat{H}_o^2 - 2\ell^3 \hat{H}_{\text{test},\tau}]^{\frac{1}{2}} \approx \hat{H}_o - (\ell^{-3}\hat{H}_o)^{-(1/2)} \hat{H}_{\text{test},\tau} (\ell^{-3}\hat{H}_o)^{-(1/2)}. \qquad (6.15)$$

Next, since the lapse functions associated with the choices τ and ϕ of time are related by $N_\phi = (p_{(\phi)} \ell^{-3})^{-1} N_\tau \approx (\ell^{-3}H_o)^{-1} N_\tau$ in the test field approximation, it follows that $(\ell^{-3}\hat{H}_o)^{-(1/2)} \hat{H}_{\text{test},\tau} (\ell^{-3}\hat{H}_o)^{-(1/2)}$ is precisely the matter Hamiltonian $\hat{H}_{\text{test},\phi}$ associated with time ϕ. Thus, in the test field approximation, the LQG evolution equation (6.12) is equivalent to

$$-i\hbar \partial_\phi \Psi(v, q_{\vec{k}}, \phi) = (\hat{H}_o - \hat{H}_{\text{test},\phi}) \Psi(v, q_{\vec{k}}, \phi). \qquad (6.16)$$

Step 2. The geometry operators $\hat{a}^4$ and $\hat{a}^6$ in the term $\hat{H}_{\text{test},\phi}$ do not carry any time dependence. (This feature descends directly form the classical Hamiltonian (6.11).) The parameters $a^4(x_0)$ and $a^6(x_0)$ in expression (6.9) of the Hamiltonian in quantum field theory in classical FLRW spacetimes on the other hand are time dependent. To bring the two theories closer, we can work in the interaction picture and set

$$\Psi_{\text{int}}(v, q_k, \phi) := e^{-(i/\hbar)H_o(\phi - \phi_o)} \Psi(v, q_{\vec{k}}, \phi) \qquad (6.17)$$

so that the evolution of Ψ_{int} is governed by $H_{\text{test},\phi}$ and of the quantum geometry operators by $\hat{H}_o$:

$$i\hbar \partial_\phi \Psi_{\text{int}}(v, q_{\vec{k}}, \phi) = \hat{H}_{\phi,\vec{k}}^{\text{int}} \Psi_{\text{int}}(v, q_{\vec{k}}, \phi) \quad \text{and} \quad \hat{a}(\phi) = e^{-(i/\hbar)\hat{H}_o(\phi - \phi_o)} \hat{a}\, e^{(i/\hbar)\hat{H}_o(\phi - \phi_o)}.$$
$$(6.18)$$

Step 3. The test field approximation also implies that the total wavefunction can be factorized: $\Psi_{\text{int}}(v, q_{\vec{k}}, \phi) = \Psi_o(v, \phi_o) \otimes \psi(q_{\vec{k}}, \phi)$. Next, to make contact with quantum field theory in *classical* FLRW spacetimes, one is led to take expectation values of the evolution equation in a semi-classical quantum geometry state $\Psi_o(v, \tau)$. We know from sections 2 and 3 that these states are sharply peaked on a solution to the effective equation. Therefore, *if we ignore fluctuations of quantum geometry*, we can replace $\langle \hat{a}^n |_\phi \rangle$ with just $\bar{a}^n(\phi)$ where $\bar{a}|_\phi$ is the expectation value of $\hat{a}|_\phi$. Then, the evolution equation (6.12) reduces to

$$i\hbar \partial_\phi \psi(q_{\vec{k}}, \phi) = \frac{\bar{N}_\phi}{2\bar{a}^3(\phi)} \big[\hat{p}_{\vec{k}}^2 + (\vec{k}^2 \bar{a}^4(\phi) + m^2 \bar{a}^6(\phi)) \hat{q}_{\vec{k}}^2 \big] \psi(q_{\vec{k}}, \phi). \qquad (6.19)$$

This is exactly the Schrödinger equation (6.9) governing the dynamics of the test quantum field on a classical spacetime with scale factor $\bar{a}$ containing a massless scalar field ϕ with momentum $\bar{p}_{(\phi)} = \bar{a}^2 \ell^3 / \bar{N}_\phi$. This is the precise sense in which the dynamics of a test quantum field on a classical background emerges from a more complete QFT on quantum FLRW backgrounds. Note however that even after our simplifications, the classical background is *not* a FLRW solution of the Einstein–Klein–Gordon equation. Rather, it is the effective spacetime $(M, \bar{g}_{ab})$ in the manner of LQC on which the quantum geometry $\Psi_o(\nu, \phi)$ is sharply peaked. But as discussed in sections 2 and 3, away from the Planck regime, $(M, \bar{g}_{ab})$ is extremely well approximated by a classical FLRW spacetime.

To summarize, quantum field theory on the (LQC-effective) FLRW spacetime emerges from LQG if one makes two main approximations: (i) $\hat{\varphi}$ can be treated as a *test* quantum field (steps 1 and 2 above) and (ii) the fluctuations of quantum geometry can be ignored (step 3). This systematic procedure also informs us on how to incorporate quantum geometry corrections to quantum field theory on classical FLRW backgrounds.

6.3. Inflationary perturbation theory in LQC

In this sub-section, we summarize a new framework for the cosmological perturbation theory that is geared to systematically take into account the deep Planck regime at and following the bounce [85]. This approach provides examples of effects that may have observational implications in the coming years because their seeds originate in an epoch where the curvature and matter densities are of Planck scale.

6.3.1. Inflation and quantum gravity. The general inflationary scenario involves a rather small set of assumptions: (i) sometime in its early history, the universe underwent a phase of rapid expansion during which the Hubble parameter was nearly constant; (ii) during this phase, the universe was well described by a FLRW solution to Einstein's equations together with small inhomogeneities which are well approximated by first order perturbations; (iii) consider the co-moving Fourier mode k_o of perturbations which has just re-entered the Hubble radius now. A few e-foldings before the time $t(k_o)$ at which k_o exited the Hubble radius during inflation, Fourier modes of quantum fields describing perturbations were in the Bunch–Davis vacuum for co-moving wave numbers in the range $\sim (10k_o, 2000k_o)$; and (iv) soon after a mode exited the Hubble radius, its quantum fluctuation can be regarded as a classical perturbation and evolved via linearized Einstein's equations. Analysis of these perturbations implies that there must be tiny inhomogeneities at the last scattering surface whose detailed features have now been seen in the CMB. Furthermore, time evolution of these tiny inhomogeneities produces large scale structures which are in excellent qualitative agreement with observations. These successes have propelled inflation to the leading place among theories of the early universe even though the basic assumptions have some *ad hoc* elements.

But as we discussed in section 6.3.1, the scenario is incomplete because it also has an in-built big-bang singularity [159]. Therefore, it is natural to ask: What is the situation in LQC which is free of the initial singularity? Does the inflationary paradigm persist or is there some inherent tension with the big bounce and the subsequent LQC dynamics that in particular exhibits a superinflation phase? If it does persist, one would have a conceptual closure for the inflationary paradigm. This by itself would be an important advantage of using LQC.

But there could be observational pay-offs as well. A standard viewpoint is that because of the huge expansion—the Bohr radius of a hydrogen atom is expanded out to 95 light years in 65 e-foldings of inflation—characteristics of the universe that depend on the pre-inflationary history will be simply washed away leaving no trace on observations in the foreseeable

future. However, this view is not accurate when one includes quantum effects. Suppose, as an example, the state of quantum fields representing cosmological perturbations is not the Bunch–Davis vacuum at the onset of inflation but contains a small density of particles. Then, because of the *stimulated emission* that would accompany inflation, this density does *not* get diluted. Moreover, this departure from the Bunch–Davis vacuum has potential observable consequences in non-Gaussianities [225]. So, it is natural to ask: Do natural initial conditions, say at the bounce, lead to interesting departures from the Bunch–Davis vacuum at the onset if inflation?

6.3.2. Strategy. To address such issues, one needs a perturbation theory that is valid all the way to the big bounce. Now, in the textbook treatment of cosmological perturbations, one begins by linearizing Einstein's equations (with suitable matter fields) and then quantizes the linear perturbations. The result is a quantum field theory on a FLRW background. As we saw in section 5, effective equations capture the key LQC corrections to general relativity. Therefore, to incorporate cosmological perturbations, one might think of carrying out the same procedure, substituting the FLRW background by a corresponding solution of the effective equations. But this strategy has two drawbacks. First, we do not have reliable effective equations for full LQG which one can linearize. Second, even if we had the full equations, it would be *conceptually incorrect* to first linearize and then quantize them because the effective equations already contain the key quantum corrections of the full theory. If one did have full LQG, the task would rather be that of simply truncating this full theory to the appropriate sector that, in the classical limit, reduces to FLRW solutions with linear perturbations[24].

In the absence of full LQG, an alternative strategy is the one that has driven LQC so far: *construct the Hamiltonian framework of the sector of general relativity of interest and then pass to the quantum theory using LQG techniques.* This strategy has been critical, in particular, in the incorporation of anisotropies. Had we tried to incorporate them perturbatively on the *effective* isotropic geometry provided by LQC, singularities would not have been resolved. Instead, we considered the Hamiltonian theory of the full anisotropic sector—say the Bianchi I model—and then carried out its loop quantization. As we saw in section 4.4, this procedure involves new elements beyond those that were used in the isotropic case and they were critical to obtaining the final, singularity-free theory. The idea behind the new framework is to use this philosophy for cosmological perturbations.

The first task then is to identify the appropriate truncation of the classical phase space. Let us begin by decomposing the full phase space of general relativity into a homogeneous and a *purely* inhomogeneous part. For this, it is simplest to assume, as in section 6.2, that the spatial manifold M is topologically $\mathbb{T}^3$. (The $\mathbb{R}^3$ topology would require us to first introduce an elementary cell, construct the theory, and then take the limit as the cell occupies full space.) As in section 6.2, let us fix spatial coordinates x^i on $\mathbb{T}^3$ and use them to introduce a fiducial triad $\mathring{e}_i^a$ and co-triad $\mathring{\omega}_a^i$. Then, every point (A_a^i, E_i^a) in the gravitational phase space Γ_{grav} can be decomposed as

$$A_a^i = c\ell^{-1}\mathring{\omega}_a^i + \alpha_a^i, \qquad \text{and} \qquad E_i^a = p\ell^{-2}\sqrt{\mathring{q}}\,\mathring{e}_i^a + \epsilon_i^a \tag{6.20}$$

where

$$c = \frac{1}{3\ell^2}\int_M A_a^i\mathring{e}_i^a\,\mathrm{d}^3\vec{x} \qquad \text{and} \qquad p = \frac{1}{3\ell}\int_M E_i^a\mathring{\omega}_i^a\,\mathrm{d}^3\vec{x}. \tag{6.21}$$

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[24] An 'in between' strategy would be to consider quantum fields satisfying the standard linearized Einstein's equations but on a background spacetime provided by the effective theory. Unfortunately, this procedure is ambiguous: because the background does not satisfy Einstein's equations, sets of linearized equations which are equivalent on a FLRW background now become inequivalent. With a judicious choice of a consistent set, this procedure may be viable. A significant fraction of the literature on cosmological perturbations in LQC is based on this hope (see e.g. section 6.4).

α_a^i and ϵ_i^a are *purely inhomogeneous* in the sense that the integrals of their contractions with $\mathring{e}_i^a$ and $\mathring{\omega}_a^i$ vanish. Matter fields can be decomposed in the same manner. This provides us a natural decomposition of the phase space into homogeneous and inhomogeneous parts: $\Gamma = \Gamma_H \times \Gamma_{IH}$.

We have to single out the appropriate sector of this theory that captures just those degrees of freedom that are relevant to the cosmological perturbation theory. For this one allows only a scalar field Φ as the matter source, and expands it as $\Phi = \phi + \varphi$ where ϕ is homogeneous and φ purely inhomogeneous, and introduces a potential $V(\Phi)$. For reasons given in section 5.3, we will set $V(\Phi) = (1/2)m^2\Phi^2$ (with $m \approx 1.21 \times 10^{-6}m_{Pl}$). We wish to treat the homogeneous fields as providing the background and inhomogeneous fields, linear perturbations. Thus, the situation is rather similar to that in our discussion of quantum fields in quantum spacetimes in section 6.2. However, there are also some key differences. First, we now wish to allow inhomogeneities *also in the gravitational field*, whence the inhomogeneous sector now contains α_a^i, ϵ_i^a in addition to φ. Furthermore, these fields are now coupled. In particular, we now have to incorporate the Gauss, the vector and the scalar constraints to first order:

$$\int_M \left(N^i C_i^{(1)} + N^a C_a^{(1)} + N C^{(1)} \right) d^3\vec{x} = 0 \qquad \forall N^i, N^a, N, \tag{6.22}$$

where N^i, N^a, N are, respectively, generators of the internal SU(2) rotations, shift and lapse fields on M. While they are arbitrary, because the constraints are linear in the purely inhomogeneous fields, only the purely inhomogeneous parts of N^i, N^a, N matter. It is simplest to solve these linearized constraints on $\alpha_a^i, \epsilon_i^a, \varphi$ and factor out by the gauge orbits generated by these constraints to pass to a reduced phase space as in [226] (see also [227–230]). Since we have ten configuration variables in (α_a^i, φ) and seven first class constraints, we are left with three true degrees of freedom: two tensor modes and a scalar mode. These can be represented as three scalar fields on M. As in section 6.3, it is simplest to pass to the Fourier space and work with the two tensor modes $q_{\vec{k}}^I$ (with $I = 1, 2$) and the scalar mode $q_{\vec{k}}$. We will often group them together as $\vec{q}_{\vec{k}}$ and denote the three conjugate momenta as $\vec{p}_{\vec{k}}$. Thus, truncated phase space of interest is given by

$$\Gamma_{Trun} = \Gamma_H \times \Gamma_{IH}^{Red}, \tag{6.23}$$

where the truncation manifests itself in the fact that the reduction of the inhomogeneous part of the phase space has been carried out using the first order truncated constraints. Dynamics on Γ_{Trunc} is governed by the Hamiltonian constraint truncated to the second order:

$$C_{N_H} = \int_M N_H(C^{(0)} + C^{(2)}) \, d^3\vec{x}, \tag{6.24}$$

where the subscript H on the lapse field emphasizes that it is a homogeneous (i.e. constant) function on M. Note that the integrand does not contain $C^{(1)}$ because its integral against a homogeneous lapse vanishes identically. To pass to quantum theory using LQC techniques, we will use harmonic time (so $N_H = a^3$). Then, as before (see section 5.3)

$$\int N_H \, C^{(0)} \, d^3\vec{x} = \frac{p_{(\phi)}^2}{2\ell^3} - \frac{3}{8\pi G \ell^3}b^2 V^2 + \frac{m^2}{2\ell^3}\phi^2 V^2 \tag{6.25}$$

while

$$\int_M N_H \, C^{(2)} d^3\vec{x} = H_\tau^{(T)} + H_\tau^{(S)} := \frac{1}{2} \sum_{I=1}^{2} \sum_{\vec{k} \in \mathcal{L}} \left[(p_{\vec{k}}^I)^2 + a^4\vec{k}^2(q_{\vec{k}}^I)^2 \right]$$

$$+ \frac{1}{2} \sum_{\vec{k} \in \mathcal{L}} \left[p_{\vec{k}}^2 + a^4\vec{k}^2 q_{\vec{k}}^2 + f(a, b, p_{(\phi)}; m)q_{\vec{k}}^2 \right] \tag{6.26}$$

has a form similar to the Hamiltonian of the matter field in section 6.2. The subscript τ is a reminder that the lapse is tailored to the harmonic time τ, the superscripts (T), (S) refer to tensor and scalar modes, and the scale factor a determines the physical volume V via $V = a^3 \ell^3$. An important difference is that the 'mass term' in the scalar mode depends on the background fields and is therefore time dependent.

Thus, the truncated phase space adapted to cosmological perturbations is given by (6.23). It has only one Hamiltonian constraint (6.24) that generates dynamics. This is the Hamiltonian theory one has to quantize using LQG techniques.

6.3.3. Quantum perturbations on quantum spacetimes. Recall that for the WMAP data, modes that are directly relevant lie in the range $\sim(10k_o, 2000k_o)$. Thus, from observational perspective, we have natural ultraviolet and infrared cutoffs, whence field theoretic issues are avoided and one can hope to proceed as in section 6.2. There is however one subtlety. Since the homogeneous part (6.25) of the constraint now contains a 'time-dependent' term $m^2\phi^2$ we face issues discussed in section 3.3. As explained there, at an abstract mathematical level, these can be handled via group averaging. However, to obtain detailed predictions via numerical simulations, with the current state of the art, one has to restrict oneself to quantum states of the background in which the bounce is dominated by kinetic energy. Now, given the $m^2\phi^2$ potential, WMAP observations lead to a very narrow window of initial conditions at the onset of inflation [83, 157]. Fortunately, we know [67, 83] that there is a wide class of states with kinetic energy domination at the bounce that meet this severe constraint. Therefore, while it is conceptually important to incorporate more general states in this analysis, even with kinetic domination one can obtain results that are directly relevant for observations.

The idea then is to use the quantization of the truncated theory to analyze dynamics of perturbations starting from the bounce. In this theory *both the background and perturbations are treated quantum mechanically* following section 6.2. Since this 'pure' quantum regime is rather abstract, it is instructive to use effective equations to develop some intuition. (For details, see [83].) They show that immediately after the bounce the background undergoes a superinflation phase, which is followed by a longer phase during which kinetic energy steadily decreases but is still larger than the potential energy. The total time for which kinetic energy dominates is of the order of 10^4 Planck units. At the end of this phase, the energy density has decreased to about $10^{-11}\rho_{\max}$. Therefore, it suffices to use the full quantum description—i.e. treat perturbations as quantum fields on a quantum geometry—only till the end of this phase. After that, one can adequately describe perturbations using standard quantum field theory on a FLRW background.

Fortunately, during the 'pure quantum phase' the background inflaton ϕ evolves monotonically. Therefore, it is appropriate to continue to interpret the quantum version of the Hamiltonian constraint (6.24)

$$-\hbar^2 \partial_\phi^2 \Psi(\nu, \vec{q}_{\vec{k}}, \phi) = \left(\hbar^2 \Theta_{(m)} - 2\ell^3 \left(\hat{H}_\tau^{(T)} + \hat{H}_\tau^{(S)}\right)\right) \Psi(\nu, \vec{q}_{\vec{k}}, \phi) \qquad (6.27)$$

as providing evolution with respect to the 'internal time' ϕ. Here, $\Theta_{(m)} = \Theta - (2\pi G\gamma m\phi\nu)^2$ where Θ is the LQC difference operator (2.45) representing the gravitational part of the constraint in the FLRW model, and, as in section 6.2, $\hat{H}_\tau^{(T)}$ and $\hat{H}_\tau^{(S)}$ depend not only on fields representing linear perturbations but also on the background operators (see (6.26)). Thus, the form of quantum constraint is the same as that in section 6.2. Our basic assumptions are incorporated by restricting oneself to any state Ψ representing a semi-classical wavefunction that is sharply peaked at a kinetic energy-dominated effective trajectory near the bounce [67] and in which the energy in perturbations is small compared to the background kinetic energy.

Then, as in section 6.2, we can make a series of controlled approximations to simplify the evolution equation.

(i) Because of kinetic energy domination, the subsequent evolution is well approximated by a first order equation analogous to (6.16):

$$-i\hbar\partial_\phi\Psi(\nu,\vec{q}_{\vec{k}},\phi) = \big(\hat{H}_o - 2\ell^3\big(\hat{H}_\phi^{(T)} + \hat{H}_\phi^{(S)}\big)\big)\Psi(\nu,\vec{q}_{\vec{k}},\phi), \qquad (6.28)$$

where the Hamiltonians on the right-hand side evolve the wavefunction in the scalar field time ϕ.

(ii) One then passes to the interaction picture in which operators (such as $\hat{a}^n \equiv \hat{V}^{n/3}/\ell^n$) referring to background geometry evolve with respect to the scalar field time.

(iii) If the evolved state factorizes as $\Psi(\nu,\vec{q}_{\vec{k}},\phi) = \Psi(\nu,\phi) \otimes \psi(\vec{q}_{\vec{k}},\phi)$, one can take the expectation value of the evolution equation w.r.t. the state $\Psi(\nu,\phi)$ of the background geometry. If furthermore the fluctuations of the background operators that appear in the definition of $\hat{H}_\phi^{(T)}$ and $\hat{H}^{(S)}$ are negligible compared to the expectation values, one obtains the familiar evolution equation, analogous to (6.19), for the evolution of the quantum state $\psi(\vec{q}_{\vec{k}},\phi)$ of perturbations in the Schrödinger picture.

The final evolution equations have the same form as the standard ones one finds in the textbook theory of quantum fields representing cosmological perturbations. However, the background fields that feature in these equations naturally incorporate both the holonomy and inverse volume corrections of LQC. More importantly, approximations involved in the passage from quantum fields representing perturbations on quantum spacetimes to quantum fields representing perturbations on curved (but LQC corrected) spacetimes are spelled out. Therefore, if numerical simulations show that they are violated, one can work at the 'higher level' before the violation occurs and still work out the consequences of this evolution (although that task will involve more sophisticated numerical work). This is a notable strength of the framework.

This candidate framework provides a systematic procedure to evolve quantum states of the background and perturbations all the way from the big bounce to the end of the kinetic dominated epoch. This endpoint lies well within the domain of validity of general relativity: as we already observed, the matter density is some 11 orders of magnitude below the Planck scale. Therefore, the subsequent quantum gravity corrections, although conceptually still interesting, will be too small for observations in the foreseeable future. But, as we emphasized in the beginning of this sub-section, since the quantum evolution begins at the bounce, quantum corrections to the standard scenario arising from the early stages could well have consequences that are observationally significant, in spite of the subsequent slow roll inflation.

An important example is the issue of what the 'correct' quantum state of perturbations is at the onset of inflation [85]. Since the onset of the slow roll phase compatible with the WMAP data occurs quite far from the Planck scale, from a conceptual viewpoint, it seems artificial to simply postulate that the state should be the Bunch–Davis vacuum there. It would be more satisfactory to select the state at the 'beginning' using physical considerations, evolve it, and show that it agrees with the Bunch–Davis vacuum at the onset of slow roll to a good approximation. But in general relativity, the beginning is the big-bang singularity and one does not know how to set initial conditions there. In bouncing scenarios—such as the one in LQC—it is natural to specify the initial quantum state of perturbations at the bounce. If the state can be specified in a compelling fashion and if it does not evolve to a state that is sufficiently close to the Bunch–Davis vacuum at the onset of the WMAP slow roll, the viability of the bouncing scenario would be seriously strained. If on the other hand the evolved state turns out to be close, but not too close, to the Bunch–Davis vacuum, there would be observable

predictions, e.g., on non–Gaussianities [225]. These possibilities call for a detailed application of the framework outlined in this section.

6.4. LQC corrections to standard paradigms

There is a large body of work investigating implications of quantum geometry in the standard cosmological scenarios based on various generalizations of effective equations. Much of the recent work in this area is geared to the inflationary and post-inflationary phases of the evolution of the universe. These investigations are conceptually important with the potential to provide guidance for full LQG. However, because there are significant variations in the underlying assumptions and degrees of precision, and because the subject is still evolving, it will take inordinate amount of space to provide an exhaustive account of these developments. Also, as one would expect, because curvature during and after inflation is very small compared to the Planck scale, the LQG corrections discussed in many of these works are too small to be measurable in the foreseeable future. Therefore, in this subsection, we will provide only a few illustrative examples to give a flavor of ongoing research in this area.

The possibility for LQG effects to leave indirect observable signatures was first considered in [231] where it was argued that the quantum geometry-induced violations of slow roll conditions could leave an imprint in the CMB at the largest scales. Since then, a wide spectrum of calculations of LQG corrections to the standard cosmological scenario have appeared in the literature and the subject has evolved significantly. In the early years, emphasis was on models *inspired* by LQC bounces and the new phase of superinflation. In more recent studies, LQC is used more systematically and underlying assumptions are also more streamlined.

A considerable effort has been made to investigate implications of the quantum geometry effects of LQC on the standard inflationary scenarios. As in the analysis of perturbations in the quasi-de Sitter inflationary paradigm, one considers a Bunch–Davis vacuum as the initial state, and studies the evolution of perturbations using effective equations that incorporate quantum gravity effects. As an example, the Fourier modes ϕ_k of tensor perturbations satisfy a second order evolution equation which is very similar to the one in the standard inflationary scenario, except for a modification in the value of frequency resulting from quantum geometry (see e.g. [72]). One then computes the correlation function for modes in the Bunch–Davis vacuum state, which yields the power spectrum. Once these modes exit the Hubble horizon, the quantum correlation function is assumed to become a classical perturbation as in the conventional scenario and is evolved using classical linearized equations. LQC effects are thus captured in the power spectrum of the perturbations, influencing both the amplitude and the spectral tilt which measures the departure from scale invariance. Such effects have been investigated in various works (see e.g. [70–73, 88, 232–242]).

These and other investigations along such lines have created interesting frameworks to make observable predictions. However, a shortcoming of these calculations is that they typically focus just on one or two aspects of quantum geometry. Definitive predictions will have to pool together all the relevant effects. Once this is done, it will become clear which effects are quantitatively significant and require further detailed analysis to arrive at reliable predictions that can be tested against observations. In addition, these explorations are of interest on the theoretical side even as they stand because they provide concrete illustrations of quantum effects one can expect in full LQG.

Broadly speaking, here are two kinds of LQG corrections that could potentially affect the evolution of cosmological perturbations. These are (i) modifications originating from expressing the field strength of the gravitational connection in terms of holonomies and (ii) corrections due to inverse volume (or scale factor) expressions in the constraint.

Holonomy corrections and cosmological perturbations. As discussed in sections 2–5, in isotropic models holonomy corrections led to a ρ^2/ρ_{max} modification of the Friedmann equation with a bounce of the background scale factor occurring at $\rho = \rho_{max}$, and a phase of super-inflation for $\rho_{max}/2 \leqslant \rho < \rho_{max}$. In the early attempts to include these modifications [68], only the fluctuations in the scalar field were considered on the unperturbed homogeneous background and, strictly speaking, the analysis was restricted just to a tiny neighborhood near the bounce. The power spectra of scalar and tensor perturbations were then computed and the scalar perturbations were shown to have a nearly scale invariant spectrum for a class of positive potentials. Scalar perturbations have also been computed under similar assumptions for multiple fluids [209].

As a next step, perturbations of geometry and matter were investigated about backgrounds provided by solutions to the effective LQC equations. Often, it is implicitly assumed that one can still use the standard general relativistic perturbation equations (but on the LQC-modified background) because one works in the era starting from the onset of slow roll inflation where the matter density and curvature are several orders of magnitude below the Planck scale. Not surprisingly, then it was found that for scalar perturbations, the corrections to the standard scenario are too small to be of interest to observational cosmology [232]. (Similar conclusions were reached in [233].) There are also more detailed and systematic calculations in which the holonomy corrections are first incorporated in an effective Hamiltonian constraint and the constraint is then perturbed to a linear order [234]. In this framework, tensor perturbations have been studied in various works [70, 72, 235, 236] in the presence of an inflationary potential[25]. These results indicate that the scenario in which perturbations are generated in the bounce followed with a standard phase of inflation is consistent with observations [72, 236]. They also point to some new interesting features. The first is a k^2 suppression of power in the infrared which is a characteristic of the bounce. Second, it has been suggested that certain statistical properties of perturbations are sensitive to the presence of a contracting phase prior to the bounce and to the bounce itself. Calculations have been performed to estimate the size of the imprints of these effects on phenomenological parameters that could be constrained or measured by the next-generation B-mode CMB experiments [73]. However, it is probably fair to say that these studies are yet to capture a unique signature of LQC which cannot be mimicked by other models.

Inverse volume corrections and cosmological perturbations. Because these corrections are simplest to study in the context of perturbations in LQC, there is a large body of literature on the subject for both scalar and tensor perturbations (see e.g. [68, 205, 238–242]). These investigations have been carried out under a variety of scenarios: approximating the asymptotic region in the deep Planck regime by a particular variation of the scale factor [239]; considering various values of j labeling representations of SU(2) used to compute the inverse volume corrections [241]; etc. The more conservative and better motivated of these assumptions do hold away from the Planck regime. But then the inverse volume corrections are too small to be of interest observationally. However, they can provide limits on the details of some LQG scenarios.

In homogeneous models, inverse volume corrections are well defined when the spatial topology is compact. In the non-compact case, they depend on the choice of the cell—the infrared regulator—used in constructing the quantum theory and seem to disappear in the limit as the regulator is removed. Therefore, strictly speaking, in the $k = 0$ case these corrections

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[25] Recently, holonomy correction on scalar perturbations have also been computed [237]. However, it is not clear whether perturbation equations satisfy all the constraints under evolution.

are interesting only if the topology is $\mathbb{T}^3$ (rather than $\mathbb{R}^3$). The topological restriction is not always spelled out and indeed it would be of interest to investigate in some detail if there are interesting regimes, *compatible with the WMAP data*, in which these corrections are significant. Irrespective of the outcome, the corrections are conceptually interesting in the $\mathbb{T}^3$ case as well as the $\mathbb{S}^3$ topology in the $k = 1$ case.

In the non-compact case, introduction of a cell is essential because of the assumption of spatial homogeneity. Therefore, one may hope that in an inhomogeneous setting, a cell would be unnecessary and the inverse volume effects would be well defined also in the non-compact topology. With this motivation, inverse scale factor modifications have been introduced by considering certain deformations of the constraint functions of general relativity that can still yield a closed algebra [243], and by postulating an effective Hamiltonian based on the results found in homogeneous models. Corrections to the linear order scalar perturbations have been computed [229]. These have been extended to the proposal of 'lattice refinement' [244] and issues of gauge invariant scalar perturbations have been analyzed [245]. Linear perturbations have also been computed for the tensor modes [71, 234, 246, 247]. More recently, inflationary observables have been studied with the goal of constraining them with the observational data [88, 248].

The notion of 'lattice refinement' has evolved over the years. In recent works, the basic idea is to decompose the spatial manifold in elementary cells and approximate the inhomogeneous configurations of physical interest by configurations which are homogeneous within any one cell but vary from cell to cell. Physically, this is a useful approximation. However, it requires a fresh input, that of the cell size (or lattice spacing), and the inverse volume effects are now sensitive to this new scale. The fiducial cell of the homogeneous model is replaced by a physical cell in which the universe can be taken to be homogeneous. This new scale may well be ultimately provided by the *actual*, physical quantum state of the universe. However, to our knowledge, a procedure to select such an inhomogeneous state has not been spelled out. Even if one somehow fixes a state, a systematic framework to arrive at this scale starting from the given state has not yet been constructed. Finally, we are also not aware of any observational guidance on what this scale should be during, say, the inflationary epoch, i.e. the epoch when one generates the perturbations in these schemes. Therefore, although the underlying idea of lattice refinement is attractive, so far there appears to be an inherent ambiguity in the size and importance of the inverse volume effects in this setting.

Finally, we will amplify on a remark in the opening paragraph of this subsection. The matter density and curvature at the onset of inflation is some 11 orders of magnitude below the Planck scale. Therefore, one would expect that quantum gravity corrections would also be suppressed by the same order of magnitude. Yet, some of the works that focus on the inflationary and post-inflationary era report corrections which are higher by several orders of magnitude. This would indeed be very interesting for quantum gravity but the mechanism responsible for these impressive enhancements needs to be spelled out to have a better understanding of and confidence in the physical relevance of these results.

Thermal fluctuations and the k = 1 model. So far our summary of LQC phenomenology has been focused on inflationary scenarios. A possible alternative to inflation is provided by the idea that the primordial fluctuations observed in CMB are of thermal origin. In conventional scenarios, this proposal faces two serious drawbacks. First, there is the horizon problem. A second difficulty is that in the general relativity-based scenarios, the spectral index of thermal fluctuations is far from being nearly scale invariant. In LQC, the first problem is naturally resolved by the bounce. In addition, the inverse volume corrections, which are well defined for the spatially closed model, lead to important modifications to the effective equation of state

[177] and affect thermodynamic relations in a non-trivial way. Preliminary investigations that incorporate these modifications indicate that the thermal spectrum can in fact be approximately scale invariant in the allowed region of parameter space [249]. Thus, the analysis reveals that the LQC corrections could revive this alternative to inflation. This possibility should be investigated further.

7. Lessons for full quantum gravity

LQC has been developed by applying the basic principles and techniques from LQG to symmetry-reduced systems. Although the symmetry reduction is quite drastic, LQC has the advantage that it provides us with numerous models in which the general quantization program underlying LQG could be completed *and, more importantly,* physics of the Planck regime could be explored in detail. Consequently, LQC has now begun to provide concrete hints for full LQG and, in some instances, for any background independent, non-perturbative approach to quantum gravity.

In recent years, LQG has advanced in two directions. On one front, the Hamiltonian theory has been strengthened by introducing matter fields which can serve as 'internal clocks and rods' (see, e.g., [92, 227, 228]) and, on the other, significant progress has been made in the path integral approach through the Engle, Pereira, Rovelli, Livine (EPRL) and Freidel–Krasnov (FK) models [99–101]. LQC sheds new light on a number of issues on both these fronts. For example, the subtleties that arose in the definition of the Hamiltonian constraint already in LQC have begun to provide guidance for the treatment of the Hamiltonian constraint in full LQG. Similarly, LQC has provided a proving ground to test the paradigm that underlies the new spin foam models. Specifically, it has been possible to examine the open issues of LQG through the LQC lens. The outcome has provided considerable support for the current strategies and, at the same time, revived or opened conceptual and technical issues in LQG. More generally, thanks to ideas that have been introduced over the past decade, any approach to quantum gravity has to take a stand on the issue of entropy bounds. Are these bounds universal, or can they be violated in the deep Planck regime? Should they be essential ingredients in the very construction of a satisfactory quantum theory of gravity or should they arise as inequalities that hold in certain regimes where quantum effects are important but an effective classical geometry still makes sense? Further, fundamental issues such as a consistent way to assign probabilities in a quantum universe can be addressed in the consistent histories paradigm. LQC provides a near ideal arena to explore such general issues as well.

In this section, we will discuss a few examples to illustrate such applications of LQC.

7.1. Physical viability of the Hamiltonian constraint

In full LQG, there is still considerable freedom in the definition of the Hamiltonian constraint. Perhaps the most unsatisfactory feature of the current status is that we do not know the physical meaning of these ambiguities. For, once the implications of making different choices are properly understood, we could rule out many of them on theoretical grounds and propose experiments to test the viability of the remaining ones. Now, these ambiguities descend even to the simple cosmological models. Therefore, it is instructive to re-examine the well-understood $k = 0$, $\Lambda = 0$ FLRW and the Bianchi I models and ask what would have happened if we had used other, seemingly simpler definitions of the Hamiltonian constraint. Such investigations have been performed and the concrete results they led to offer some guidance for creating viability criteria in the full theory.

The first criterion is to demand internal coherence in the following sense: physical predictions of the theory must be independent of the choices of regulators and fiducial structures that may have been used as mathematical tools in its construction. Let us begin with the $k = 0$, $\Lambda = 0$ FLRW model. In classical general relativity, spatial topology plays no role in the sense that the reduced field equations are the same whether spatial slices are compact with $\mathbb{T}^3$ topology or non-compact with $\mathbb{R}^3$ topology. However, as we emphasized earlier, in the non-compact case the symplectic structure, the Hamiltonian and the Lagrangian all diverge because of spatial inhomogeneity. Since these structures are needed in canonical and path integral quantization, this divergence impedes the passage to quantum theory. As we saw in section 2, a natural strategy is to introduce an infrared regulator, i.e. a cell $\mathcal{C}$, and restrict all integrations to it. But we have the rescaling freedom $\mathcal{C} \rightarrow \beta^3 \mathcal{C}$ where β is a positive real number. How do various structures react to this change? At the classical level, we found in section 2.1 that although the symplectic structure and the Hamiltonian transform non-trivially, physics—the equations of motion for geometry and matter fields—are all invariant under the rescaling.

What about the quantum theory? Now the dynamics is governed by the Hamiltonian constraint. The expression of the Hamiltonian constraint contains the gravitational connection c. However, since only the holonomies of these connections, rather than the connections themselves, are well-defined operators, the systematic quantization procedure leads us to replace c by $\sin \bar{\mu} c / \bar{\mu}$ where $\bar{\mu}$ can be thought of as the 'length' of the line segment along which the holonomy is evaluated. Now, in the older treatments, $\bar{\mu}$ was set equal to a constant, say μ_o (see, e.g., [37, 40, 43, 45, 112, 193]). With this choice, the Hamiltonian constraint becomes a difference operator with uniform steps in $p \sim a^2$. The resulting quantum constraint is non-singular at $a = 0$ [45] and evolution of states which are semi-classical at late times leads to a bounce [52].

However, a closer examination shows that this dynamics has several inadmissible features. First, the energy density at which bounce occurs scales with the change $\mathcal{C} \rightarrow \beta^3 \mathcal{C}$ in the size of the fiducial cell. As an example, for the massless scalar field, the density at bounce is given by [52]

$$\rho_{\max}^{(\mu_o)} = \left(\frac{2^{1/3} 3}{8 \pi G \gamma^2 \lambda^2} \right)^{3/2} \frac{1}{p_{(\phi)}}, \tag{7.1}$$

where, as before, λ^2 is the area gap of LQG. Keeping the fiducial metric fixed, under the rescaling of the cell $\mathcal{C} \rightarrow \beta^3 \mathcal{C}$, we have $p_{(\phi)} \rightarrow \beta^3 p_{(\phi)}$ and hence $\rho_{\max}^{(\mu_o)} \rightarrow \beta^{-3} \rho_{\mathrm{crit}}^{(\mu_o)}$. But the density at the bounce should have a direct physical meaning that should not depend on the size of the cell. Moreover, if we were to remove the infrared regulator in this final result, i.e. take the limit in which $\mathcal{C}$ occupies the full $\mathbb{R}^3$, we would find $\rho_{\max}^{(\mu_o)} \rightarrow 0$! This severe drawback is also shared by more general matter [54]. The effective Hamiltonian corresponding to this μ_o quantization implies

$$\rho = \frac{3 \sin^2(\mu_o c)}{8 \pi \gamma^2 G \lambda^2 |p|} \tag{7.2}$$

for general matter sources. Since $|p| \rightarrow \beta^2 |p|$, and $c \rightarrow \beta c$, ρ has a complicated rescaling property. But ρ, the physical density, cannot depend on the choice of the size of the cell $\mathcal{C}$! Thus, the μ_o-scheme for constructing the Hamiltonian constraint, simple as it seems at first, fails the theoretical criterion of 'internal coherence' we began with.

But it also has other limitations. One can bypass the theoretical coherence criterion by restricting oneself to the spatially compact $\mathbb{T}^3$ topology where one does not need a fiducial cell at all. But now we still have a problem with the quantum gravity scale predicted by the theory:

with a massless scalar field source, from equation (7.1) one finds that for large values of $p_{(\phi)}$, the density $\rho_{\max}^{(\mu_o)}$ at the bounce is very small. To see how small, let us recall an example from section 3.3.2. Consider a hypothetical $k = 0$, $\Lambda = 0$ universe with $\mathbb{T}^3$ topology and massless scalar field. Suppose that when its radius equals the observable radius of our own universe at the CMB time, it has the same density as our universe then had. For such a universe $p_{(\phi)} \approx 10^{126}$ in Planck units, so the density at the bounce would be $\rho_{\max}^{(\mu_o)} \approx 10^{-32}$ gm cm^{-3}!

A third problem with μ_o quantization is the lack of correct infrared limit in a regime well away from the bounce in which the spacetime curvature is small. This is most pronounced when matter violates strong energy condition, as in the inflationary scenario. For such matter, μ_o quantization predicts that the expanding $k = 0$ universe will recollapse at a late (but finite) time, in qualitative disagreement with general relativity at low densities [54] (see also [250]) and showing incompatibility with the inflationary scenario [251].

Thus, irrespective of the choice of spatial topology, μ_o quantization suffers from severe problems both in the ultraviolet and infrared regimes. These problems also arise in other proposals for quantization of the Hamiltonian constraint. One such proposal results from an attempt to put the constraint operator in LQC in a more general setting [244]. In this proposal, one effectively works with a more general pair of canonical variables for the gravitational phase space

$$P_g = c|p|^m \qquad \text{and} \qquad g = \frac{|p|^{1-m}}{1-m} \tag{7.3}$$

and writes the gravitational part of the constraint as a difference operator with uniform steps in g. The μ_o scheme now corresponds to the specific choice $m = 0$. For the FLRW model with a massless scalar field, following the procedure used in LQC, one can derive the maximum density at the bounce for any m to obtain [54]

$$\rho_{\max}^{(\mu_m)} = \frac{3}{8\pi G \gamma^2 \lambda^2} \left(\frac{8\pi G}{6} \gamma^2 \lambda^2 p_{(\phi)}^2 \right)^{(2m+1)/(2m-2)}. \tag{7.4}$$

Thus, except for $m = -1/2$, the energy density at bounce depends on $p_{(\phi)}$ and hence suffers from the same problems which plague μ_o quantization. In addition, the analysis of different m parametrizations shows that various quantization ambiguities disappear in the continuum limit only if $m = -1/2$ [252].

The $m = -1/2$ choice corresponds *precisely* to the 'improved dynamics [53] discussed at length in sections 2 and 3. This scheme is free from all the problems discussed above. The density at the bounce predicted by the effective theory is an absolute constant $\rho_{\max} \approx 0.41 \rho_{\rm Pl}$; not only is it insensitive to the choice of $\mathcal{C}$ but it is also the absolute upper bound of the spectrum of the (time-dependent) density operator $\hat{\rho}|_\phi$ in the quantum theory. It agrees with general relativity at weak curvatures even when one includes a cosmological constant or inflationary potentials violating the strong energy condition. Finally, it was arrived at not by an *ad hoc* prescription but by using a systematic procedure (discussed in section 2.5.2).

Ambiguities in the quantization of the Hamiltonian constraint have also been studied for the Bianchi I model. There is an operator that meets all the viability criteria discussed above in the FLRW case [3]. It was presented in section 4.4 and its effective dynamics was discussed in section 5.4.1. This choice of the Hamiltonian constraint leads to universal bounds on energy density and the shear scalar.

This is in striking contrast with the results from an earlier quantization of the Bianchi I model [162], based on an 'obvious' generalization, $\bar{\mu}_i \propto 1/\sqrt{|p_i|} \propto 1/a_i$, of the successful $\bar{\mu}$ scheme in the FLRW model [53]. Again this seemingly straightforward strategy does lead to a theory but one with severe limitations [164, 165, 253]. First, for the $\mathbb{R}^3$ topology, one

again needs a cell $\mathcal{C}$ and the rescaling freedom is now enlarged to $L_i \to \beta_i L_i$ where L_i are the lengths of $\mathcal{C}$ with respect to a fiducial metric. Under these rescalings, we have $c_1 \to \beta_1 c_i$ and $p_1 \to \beta_2 \beta_3 p_1$, etc. If the three β_i are unequal, the 'shape' of the cell changes and even the effective constraint fails to be invariant under such rescalings [164, 165]:

$$C_{\text{grav}}^{(\text{eff})} = -\frac{1}{8\pi G\gamma^2}\left(\frac{\sin(\bar{\mu}_1 c_1)\sin(\bar{\mu}_2 c_2)}{\bar{\mu}_1 \bar{\mu}_2} p_1 p_2 + \text{cyclic terms}\right), \tag{7.5}$$

where $\bar{\mu}_i = \lambda/\sqrt{p_i}$.[26] Second, on the constraint surface of this effective theory, one obtains

$$\rho = \frac{1}{8\pi G\gamma^2 \Delta \ell_{\text{Pl}}^2}\left(\frac{\sqrt{|p_1||p_2|}}{|p_3|}\sin(\bar{\mu}_1 c_1)\sin(\bar{\mu}_2 c_2) + \text{cyclic terms}\right). \tag{7.6}$$

Note that, in comparison to equation (5.18)—the effective equation that follows from the quantum theory summarized in section 4.4—here the trignometric functions of connection are multiplied with terms containing p_i. As a result the energy density—a physical quantity that cannot depend on the choice of a cell—fails to be invariant under all permissible rescalings of $\mathcal{C}$. One may attempt to avoid this problem by restring oneself only to compact topology, $\mathbb{T}^3$. However, ultraviolet problems still remain because ratios such as $\sqrt{|p_1||p_2|}/|p_3|$ grow unboundedly when one of the scale factors approaches zero or infinity. For generic initial conditions, it is possible for evolution in the Bianchi I model to lead to such regimes, making the energy density increase without a bound. Thus, again, an apparently straightforward avenue to the construction of the Hamiltonian constraint leads to a theory that is untenable both because it fails the 'internal coherence' criterion in the non-compact case, and because it has an undesirable ultraviolet behavior irrespective of topology.

These examples illustrate that even though *a priori* it may seem that there is considerable freedom in defining the Hamiltonian constraint, one can introduce well motivated criteria that can serve as Occam's razor. The two LQC examples we discussed bring out four important points: (i) internal coherence, a good ultraviolet behavior and the requirement that quantum dynamics should not lead to large deviations from general relativity in tame regimes, already constitute powerful constraints; (ii) it is important to work out a few basic consequences of the proposed theory and not be satisfied only with a mathematically consistent definition of the Hamiltonian constraint; (iii) seemingly natural choices in the definition of the Hamiltonian constraint can lead to theories that are not physically viable; and (iv) although the totality of requirements may seem oppressively large at first, they *can be* met if one follows a well-motivated path that is conceptually well grounded. Indeed, recent investigations of parametrized field theories suggest that a suitable analog of the $\bar{\mu}$ scheme of [3, 53] is likely to be necessary also in full LQG [254].

Remark. In addition to the above considerations, another viability criterion arises from investigating stability of the quantum difference equation and conditions under which it leads to a semi-classical behavior. In the Bianchi I model, for example, the quantization proposed in [140] leads to an unstable difference equation and is therefore problematic [255]. These methods provide a complimentary way to narrow down the quantization ambiguities.

7.2. LQG with a scalar field

The fact that the massless scalar field provides a global relational time variable in LQC greatly simplifies the task of solving the constraint and constructing the physical sector of the theory.

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[26] One may be tempted to restrict the fiducial cell to be 'cubical' to avoid this rescaling problem. However, the distinction between cubical and non-cubical cells is unphysical since for *any* non-cubical fiducial cell, one can always choose a fiducial flat metric such that the cell is cubical and vice versa.

It also enables one to introduce convenient Dirac observables and extract the physics of the deep Planck regime. It is therefore natural to ask if this scheme can be extended to full LQG. In fact a proposal along these lines was made already in the nineties [93, 94]. However, there was no significant follow-up because of two reasons. First, the deparametrization procedure in [93] simply assumed that the scalar field would serve as a good time variable. In the classical theory, this amounts to assuming that every solution of Einstein–Klein–Gordon system admits a foliation by space-like surfaces on each leaf of which the scalar field ϕ is constant. This cannot hold in the spatially non-compact (e.g. asymptotically flat) context because the total energy of such a scalar field would have to diverge (for physically interesting lapse fields). Even in the spatially compact context, it appears implausible that the assumption will hold in the full classical theory. The second problem was that, at that time, LQG kinematics had not been fully developed to have sufficient confidence in the then treatment of quantum constraints. Advances in LQG [227, 228] and especially LQC [53] led to a re-examination of the proposal and recently it was revived in a somewhat different and sharper form [92]. In this subsection, we will summarize the main ideas of this work.

Let us begin by recalling the classical Hamiltonian framework of this model. Fix a compact 3-manifold M. The phase space Γ of the Einstein–Klein–Gordon system consists of quadruples $\left(A_a^i, E_i^a; \phi, p_{(\phi)}\right)$. They are subject to the Gauss, the diffeomorphism and the Hamiltonian constraints. The Gauss constraint does not play an important role and can be handled both in the classical and quantum theories in a standard fashion [26, 35, 36]. Let us therefore focus on the other two constraints. They are usually written as

$$C_a := C_a^{\text{grav}} + p_{(\phi)} D_a \phi \approx 0$$
$$C := C_{\text{grav}} + \frac{1}{2} \frac{p_{(\phi)}^2}{\sqrt{q}} + \frac{1}{2} q^{ab} D_a \phi D_b \phi \sqrt{q} \approx 0, \tag{7.7}$$

where the label 'grav' refers to the gravitational parts of the constraints whose explicit form will not be needed here. Note that $C_a, C_a^{\text{grav}}, C, C_{\text{grav}}$ are all differentiable functions on Γ whence their Hamiltonian vector fields are well defined everywhere.

The first observation is that the surface $\bar\Gamma$ in Γ where these constraints are satisfied is the same as the surface on which the following constraints hold [94]:

$$C_a := C_a^{\text{grav}} + p_{(\phi)} D_a \phi \approx 0$$
$$C' := C_{\text{grav}} + \frac{1}{2} \frac{p_{(\phi)}^2}{\sqrt{q}} \mp \sqrt{C_{\text{grav}}^2 - q^{ab} C_a^{\text{grav}} C_b^{\text{grav}}} \approx 0, \tag{7.8}$$

where the quantity under the square root is guaranteed to be non-negative in a neighborhood of $\bar\Gamma$. In what follows, we restrict to this neighborhood in classical considerations. In this neighborhood, the new constraint function C' is also differentiable everywhere on the phase space *except* on the surface Γ_{sing} on which $C_{\text{grav}}^2 - q^{ab} C_a^{\text{grav}} C_b^{\text{grav}}$ vanishes somewhere on M. Away from Γ_{sing}, one can calculate the Poisson brackets between these constraints. The Poisson brackets of the Gauss and the diffeomorphism constraints with all constraints are the standard ones. What about the Hamiltonian constraints? Recall that the Poisson brackets between $C(x)$ do not vanish and, moreover, the right-hand side of the brackets involves *structure functions* rather than structure constants. In the rich literature on quantum geometrodynamics, this complication has often been referred to as the principal obstacle in canonical quantization of the theory. The situation is entirely different for $C'(x)$ [94]: *the Poisson bracket among the new Hamiltonian constraints $C'(x)$ vanish identically*! This is a major simplification.

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The next key observation [92, 94] is that the scalar constraint $C' \approx 0$ in (7.8) is well tailored for deparametrization: it is of the form

$$p_{(\phi)}^2 = \sqrt{q}\left[-C_{\text{grav}} \pm \sqrt{C_{\text{grav}}^2 - q^{ab}C_a^{\text{grav}}C_b^{\text{grav}}}\,\right], \tag{7.9}$$

where the right-hand side contains phase space functions that depend *only on the gravitational fields*. Thus, it is exactly of the form we encountered in homogeneous LQC models with a massless scalar field. Therefore, as in LQC, one can hope to pass to the quantum theory by imposing, in addition to the quantum Gauss and the diffeomorphism constraints which have been studied extensively [26, 34–36], the (infinite family of) quantum Hamiltonian constraints:

$$\hbar^2 \frac{\delta^2 \Psi(A, \phi)}{\delta\phi(x)^2} = -\Theta_{\text{LQG}}(x)\Psi(A, \phi), \tag{7.10}$$

where Θ_{LQG} is to be the quantum operator corresponding to the right-hand side of (7.9). After making a key observation that elements necessary to arrive at a rigorous definition of Θ_{LQG} are already in place in the LQG literature, a concrete candidate is proposed in [92]. The next idea is to construct the physical Hilbert space by taking the positive square root of (7.10) as in LQC and introduce relational Dirac observables along the lines of the LQC observables $\hat{V}|_\phi$ and $\hat{\rho}|_\phi$ (defined in sections 2 and 3). (Even explicit formulas for such Dirac observables are available but their physical meaning is often unclear.) This is the setup necessary to extract physics from the quantum evolution and check if it satisfies viability criteria such as those outlined in section 7.1. Since there is considerable freedom in defining Θ_{LQG}, these checks are essential to streamline and reduce the choices. Developments in cosmology can provide guidance for this task and also supply an anchor to interpret the resulting quantum theory.

The potential for a strong interplay between this program and LQC is illustrated by the following considerations. Let us first briefly return to the classical theory. Note first that in arriving at (7.9) from (7.7), spatial derivatives of ϕ are *not* set equal to zero; one does not even assume that spacetimes of interest admit a space-like foliation by $\phi = \text{const}$ surfaces. Nonetheless, there is an interesting result. A large portion $\bar{\Gamma}_{\text{reg}}$ of Γ admits a positive lapse function N such that if one starts at a point on $\bar{\Gamma}_{\text{reg}}$ at which ϕ is constant on M, then along the Hamiltonian vector field of $C'(N)$, the scalar field ϕ remains constant on M but increases monotonically. Thus, the solution to the Einstein–Klein–Gordon system determined by the initial point in $\bar{\Gamma}_{\text{reg}}$ does admit a space-like foliation by $\phi = \text{const}$ surfaces at least locally, i.e. as long as the dynamical trajectory generated by $C'(N)$ remains in $\bar{\Gamma}_{\text{reg}}$.[27] The homogeneous sector $\bar{\Gamma}_{\text{hom}}$ of $\bar{\Gamma}$ (on which all fields are homogeneous) is of course in $\bar{\Gamma}_{\text{reg}}$ and, if the initial point lies on $\bar{\Gamma}_{\text{hom}}$ then the dynamical trajectory never leaves it. Therefore, it is reasonable to assume that in an open neighborhood of homogeneous solutions to the Einstein–Klein–Gordon system, spacetimes would admit a space-like foliation by $\phi = \text{const}$ surfaces for a long time (as measured by ϕ), and this time would grow as the strength of inhomogeneities decreases.

Therefore, it would be helpful to apply this LQG framework to the cosmological perturbation theory discussed in section 6.3. Specifically, it would be helpful to expand the right-hand side of constraint (7.9) around a FLRW background and then pass to the quantum theory, focusing in the first step just on the tensor modes (thereby avoiding gauge issues and the technically more complicated form of the perturbed part of the Hamiltonian constraint). The procedure outlined in section 6.3 may provide valuable guidance in removing ambiguities in the definition of the operator Θ_{LQG}. If the mathematical program outlined

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[27] $\bar{\Gamma}_{\text{reg}}$ is the portion of the constraint surface which excludes points of Γ_{sing} *and* has the property that $p_{(\phi)}$ is nowhere vanishing on M. The lapse is given by $N = \sqrt{q}/p_{(\phi)}$; it is 'live', i.e. depends on the dynamical variables. Of course all these arguments are at the same level of rigor as is commonly used in the Hamiltonian framework in general relativity; they are not rigorous in the sense of functional analysis used in PDEs.

in [92] is completed, LQC would also play a key role in the physical interpretation of that theory. The most 'secure' interpretation is likely to come from states that are sharply peaked at homogeneous geometries in the regime in which general relativity is a good approximation. The quantum Hamiltonian equation would naturally provide an evolution of these states in the internal time ϕ. Results from LQC suggest natural, physically important questions that this theory could address. Is the singularity still resolved in spite of the presence of an infinite number of degrees of freedom which are now treated non-perturbatively? Do LQC results correctly capture the qualitative features of the Planck scale physics? Thus, the cosmological context provides a natural home for this sector of LQG which is poised to make technical advances in the coming years.

7.3. Spin foams

The goal of spin foam models (SFM) is to provide a viable path integral formulation of quantum gravity. Because there is no background spacetime, the framework underlying this program has certain novel features that are not shared by path integral formulations of familiar field theories in Minkowski space. LQC offers a simple context to test the viability of these novel elements [102–105, 256]. Conversely, SFM offer a possible avenue to arrive at LQC starting from full LQG [106–108].

7.3.1. Conceptual setting.
As we discussed in section 1, the kinematical framework of full LQG is well established. A convenient basis in $\mathcal{H}_{\text{kin}}^{\text{total}}$ is provided by the so-called spin network states [26, 35, 36, 135, 136]. The key challenge is to extract physical states by imposing quantum constraints on spin networks. Formally this can be accomplished by the group averaging procedure which also provides the physical inner product [26, 34–36, 48]. From the LQG perspective, the primary goal of SFMs is to construct a path integral to obtain Green's function—called the *extraction amplitude*—that captures the result of group averaging. As explained in section 3.5, in the timeless framework of quantum gravity, the extraction amplitude determines the full content of quantum dynamics, just as the transition amplitudes do in the familiar field theories in Minkowski spacetimes.

Heuristically, the main idea behind this construction can be summarized as follows [95]. Consider a 4-manifold M bounded by two 3-surfaces, S_1 and S_2, and a triangulation $\mathcal{T}$ of M. One can think of S_1 as an 'initial' surface and S_2 as a 'final' surface. One can fix a spin network on each of these surfaces to specify an 'initial' and a 'final' quantum 3-geometry. A quantum 4-geometry interpolating between the two is captured in a 'colored' 2-complex $\mathcal{T}^\star$ dual to the simplicial decomposition where the coloring assigns to each 2-surface in $\mathcal{T}^\star$ a half-integer j and to each edge an intertwiner. The idea is to obtain the extraction amplitude by summing first over all the colorings for a given $\mathcal{T}$, and then over triangulations, keeping the boundary states fixed. The second sum is often referred to as the *vertex expansion* because the Mth term in the series corresponds to a $\mathcal{T}^\star$ with M vertices (each of which corresponds to a simplex in $\mathcal{T}$). Since each colored $\mathcal{T}^\star$ specifies a quantum geometry, the sum is regarded as a path integral over physically appropriate 4-geometries.

Group field theory (GFT) provides a conceptually distinct method to obtain the same vertex expansion. The underlying idea is that gravity is to emerge from a more fundamental theory based on abstract structures that, to begin with, have nothing to do with spacetime geometry. Examples are matrix models for two-dimensional gravity and their extension to 3-dimensions—the Boulatov model [96]—where the basic object is a field on a group manifold rather than a matrix. The Boulatov model was further generalized to four-dimensional gravity [26, 97, 98]. The resulting theory is again formulated on a group manifold, rather than

spacetime. However, as in familiar field theories, its Lagrangian has a free and an interaction term, with a coupling constant $\underline{\lambda}$. In the perturbation expansion, the coefficient of $\underline{\lambda}^M$ turns out to be Mth term in the spin foam vertex expansion.

Over the last 3–4 years SFM have witnessed significant advances (see, e.g., [99–101]). In particular, it was shown that, thanks to the discreteness of eigenvalues of the area operator, the sum over colorings has no ultraviolet divergences. More recently, it has been argued that the presence of a *positive* cosmological constant naturally leads to an infrared regularization [257]. These are striking results. However, a number of issues still remain because so far a key ingredient in the spin foam sum over histories—the vertex amplitude—has not been systematically derived following procedures used in well-established field theories or from a well-understood Hamiltonian dynamics. More importantly, because the number of allowed triangulations grow *very* rapidly with the number of vertices, and a compelling case for restricting the sum to a well-controlled subset is yet to be made, the issue of convergence of the vertex expansion is wide open. Finally, there is also a conceptual tension between the SFM and GFT philosophies. Do the $\underline{\lambda}^M$ factors in the perturbative expansion of GFT merely serve as book-keeping devices, to be set equal to 1 at the end of the day to recover the SFM extraction amplitude? Or, is there genuine, new physics in the GFT at lower values of $\underline{\lambda}$ which is missing in the spin foam program? For this to be a viable possibility, $\underline{\lambda}$ should have a direct physical interpretation in the spacetime picture. What is it?

These and other open issues suggest that the currently used SFM and GFT models will evolve significantly over the next few years. Indeed this seems likely because, thanks to the recent advances, this community has grown substantially. Therefore, at this stage, it seems appropriate to examine only of the underlying, general paradigms rather than specifics of the models that are being pursued. Is it reasonable to anticipate that the 'correct' extraction amplitude will admit a vertex expansion? Are there physical principles that constrain the histories one should be summing over? Can symmetry-reduced models shed some light on the physical meaning of $\underline{\lambda}$ of GFT? LQC has turned out to be an excellent setting to analyze these general issues.

7.3.2. Cosmological spin foams.   For definiteness, let us consider the Bianchi I model [105] with a massless scalar field as in section 4.4. A convenient basis in the kinematical Hilbert space $\mathcal{H}_{\text{kin}}^{\text{total}}$ is now given by $|v, \vec{l}, \phi\rangle$ where $\vec{l} = l_1, l_2$ are the eigenvalues of the anisotropy operators and, as before, v and ϕ of the volume and scalar field operators. This is the LQC analog of the spin network basis of LQG. As in section 3.5, the group averaging procedure [34, 48, 49] provides us with the extraction amplitude

$$\mathcal{E}(v_f, \vec{l}_f, \phi_f; v_i, \vec{l}_i, \phi_i) := \int_{-\infty}^{\infty} \mathrm{d}\alpha \langle v_f, \vec{l}_f, \phi_f | \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\alpha\hat{C}} | v_i, \vec{l}_i, \phi_i\rangle, \qquad (7.11)$$

where $\hat{C} = -\hbar^2(\partial_\phi^2 + \Theta_{(I)})$ is the full Hamiltonian constraint of the Bianchi I model. (As in section 3.5 for simplicity of notation, we have chosen not to write explicitly the θ function that restricts to the positive part of the spectrum of $\hat{p}_{(\phi)}$.) Again, since the integrated operator is heuristically '$\delta(\hat{C})$', the amplitude $\mathcal{E}(v_f, \vec{l}_f, \phi_f; v_i, \vec{l}_i, \phi_i)$ satisfies the Hamiltonian constraint in both sets of its arguments. Consequently, it serves as Green's function that maps states $\Psi_{\text{kin}}(v, \vec{l}, \phi)$ in the kinematical space $\mathcal{H}_{\text{kin}}^{\text{total}}$ to states $\Psi_{\text{phys}}(v, \vec{l}, \phi)$ in $\mathcal{H}_{\text{phy}}$ through a convolution

$$\Psi_{\text{phys}}(v, \vec{l}, \phi) = \sum_{v', \vec{l}'} \int \mathrm{d}\phi' \mathcal{E}(v, \vec{l}, \phi; v', \vec{l}', \phi') \Psi_{\text{kin}}(v', \vec{l}', \phi') \qquad (7.12)$$

and enables us to write the physical inner product in terms of the kinematical:

$$(\Phi_{\text{phys}}, \Psi_{\text{phys}}) := \sum_{v, \vec{l}, v', \vec{l}'} \int d\phi \, d\phi' \bar{\Phi}_{\text{kin}}(v, \vec{l}, \phi) \mathcal{E}(v, \vec{l}, \phi; v', \vec{l}', \phi') \Psi_{\text{kin}}(v', \vec{l}' \, \phi'). \tag{7.13}$$

As in section 3.5, one can just follow the *mathematical* procedure first given by Feynman [150] by regarding $\mathcal{E}(v_f, \vec{l}_f, v_f; v_i, \vec{l}_i, \phi_f)$ as a transition amplitude for the initial state to evolve to the final one in the 'unit time interval' during the evolution generated by a fictitious 'Hamiltonian' $\alpha \hat{C}$. Again, the 'time interval' and the 'Hamiltonian' are fictitious mathematical constructs because in the physical example under consideration, we are in the timeless framework and $\hat{C}$ is the constraint operator, rather than the physical Hamiltonian. There is however one difference from section 3.5. To make contact with spin foams, one has to remain in the configuration space with paths representing *discrete quantum geometries*: since we are not interested in semi-classical considerations, there is no need to express the extraction amplitude as a sum over classical phase space paths.

In the Feynman procedure, one first divides the 'unit time interval' into a large number N of segments, each of length $\epsilon = 1/N$, by introducing $N - 1$ decompositions of identity $|v_{N-1}, \vec{l}_{N-1}\rangle\langle\vec{l}_{N-1}, v_{N-1}| \ldots |v_1, \vec{l}_1\rangle\langle\vec{l}_1, v_1|$, between the final and initial states in the expression of the amplitude $\mathcal{E}$. This enables one to write $\mathcal{E}$ as a sum over discrete quantum histories. The key new step is to reorganize this sum by grouping together all paths that contain *precisely N* volume transitions [102, 103]. Then, after taking the limit $N \to \infty$, one obtains

$$\mathcal{E}(v_f, \vec{l}_f, \phi_f; v_i, \vec{l}_i, \phi_i) = \sum_{M=0}^{\infty} \left[\sum_{v_{M-1}, \ldots, v_1} A(v_f, v_{M-1}, \ldots, v_1, v_i; \vec{l}_f, \vec{l}_i; \phi_f, \phi_i) \right]$$

$$\equiv \sum_{M=0}^{\infty} A(M). \tag{7.14}$$

The partial amplitude $A(v_f, v_{M-1}, \ldots, v_1, v_i; \vec{l}_f, \vec{l}_i; \phi_f, \phi_i)$ is obtained by summing over all paths in which the volume changes from v_i to v_1, v_1 to v_2, ..., v_{M-1} to v_f. These ordered sequences of volume transitions can occur at any values of ϕ and can be accompanied by arbitrary changes in anisotropies $\vec{l}$ subject only to the initial and final values, $\phi_i, \vec{l}_i$ and $\phi_f, \vec{l}_f$. Still the amplitude $A(v_f, v_{M-1}, \ldots, v_1, v_i; \vec{l}_f, \vec{l}_i; \phi_f, \phi_i)$ is a well-defined, finite expression which can be expressed in terms of the matrix elements of $\Theta_{(I)}$. In the final expression, $A(M)$ is the contribution to the extraction amplitude arising from *precisely M* volume transitions, subject just to the initial and final conditions. Thus, fixing M is analogous to fixing the number of vertices in SFM and summing over intermediate volumes and anisotropies is analogous to summing over 'colorings' (spins and intertwiners) [105]. In this sense, (7.14) is the analog of the vertex expansion of SFM.

There is also a neat analog of the GFT perturbative expansion of the extraction amplitude. The idea is to split $\Theta_{(I)}$ as $\Theta_{(I)} = \hat{D} + \hat{K}$ where $\hat{D}$ is diagonal in the volume basis $|v\rangle$ and $\hat{K}$ is *purely* off-diagonal, and regard $\hat{D}$ as the 'main part' of the constraint and $\hat{K}$ as a 'perturbation'. Again, this is only a mathematical step that allows us to use the well-developed framework of perturbation theory. To highlight our intention, let us introduce a coupling constant $\underline{\lambda} \in (0, 1)$ and consider, in place of $\hat{C}$, the operator $\hat{C}_{\underline{\lambda}} = -\hbar^2(\partial_\phi^2 + \hat{D} + \underline{\lambda}\hat{K})$. Then, we can use the standard perturbation theory in the interaction picture to calculate the transition amplitude $\mathcal{E}_{\underline{\lambda}}$. One is directly led to

$$\mathcal{E}_{\underline{\lambda}}(v_f, \vec{l}_f, \phi_f; v_i, \vec{l}_i, \phi_i) = \sum_{M=0}^{\infty} \underline{\lambda}^M A(M), \tag{7.15}$$

where the coefficients $A(M)$ are *exactly* the same as in (7.14). Furthermore, this perturbative treatment enables one to extract the meaning of truncating the expansion after, say, first M_o terms as is done in practice in spin foam calculations. One can show that the resulting truncated series satisfies the Hamiltonian constraint to order $O(\lambda^{M_o})$. To recover the full extraction amplitude of direct physical interest, one has to simply set $\underline{\lambda} = 1$ in (7.15). Thus, equation (7.15) of LQC is analogous to the expression of the transition amplitude obtained in GFT.

GFT considerations naturally led us to ask if there is a physical meaning to the generalization $\mathcal{E}_{\underline{\lambda}}$ of the extraction amplitude for $\underline{\lambda} \neq 1$. This issue as been analyzed in detail in the isotropic case and, somewhat surprisingly, the answer turns out to be in the affirmative [103]. Suppose, as in our discussion so far, we are interested in LQC/SFM with $\Lambda = 0$ but let us allow a cosmological constant Λ in the GFT-like perturbation series. Then, one can show that the $\Lambda = 0$ LQC/SFM theory is unitarily equivalent to LQC/GFT with $\Lambda = 3(1 - \underline{\lambda})/2\gamma^2\, \mathfrak{l}_o{}^2$ [103]! This fact leads us to an intriguing possibility. From a GFT perspective, the 'correct' physical interpretation of the $\underline{\lambda}$-theory would be that it has a non-zero cosmological constant. At weak coupling, i.e. $\underline{\lambda} \approx 0$, we have $\Lambda \sim 1/\ell_{\mathrm{Pl}}^2$. This is just as one may expect from the 'vacuum energy considerations' in Minkowski space. As $\underline{\lambda}$ increases and approaches the SFM value $\underline{\lambda} = 1$, we have $\Lambda \to 0$. Now, $\underline{\lambda}$ is expected to run in GFT. So, Λ would seem to run from its perturbative value $\Lambda \sim 1/\ell_{\mathrm{Pl}}^2$ to $\Lambda \sim 0$ (from above). If the flow reached close to $\underline{\lambda} = 1$ but not exactly $\underline{\lambda} = 1$, GFT would say that there is a small positive Λ. This is only a speculative scenario because it mixes precise results in the isotropic LQC model with expectations in the full GFT. It is nonetheless interesting because it provides an attractive paradigm to 'explain' the smallness of the observed value cosmological constant using GFT.

To summarize, the Hamiltonian LQC provides a well-defined, closed expression of the extraction amplitude. Therefore, one can use it to probe questions raised in sections 7.3.1. We found that one can simply rewrite it as a discrete series (7.14) mimicking the vertex expansion of SFM or as a perturbation series (7.15) mimicking the expression of the extraction amplitude in GFT. (The only assumption made in arriving at these expressions is that the infinite sum $\sum_M$ can be interchanged with the integration over α in (7.11).) In this sense, cosmological spin foams provide considerable support for the general paradigm underlying SFM and GFT. Finally, here we worked with the timeless framework. However, we can also deparameterize the theory using the scalar field as a global, relational time variable as in section 4.4. Then, the constraint is reduced to a standard Schrödinger equation with ϕ as time and one can meaningfully speak of transition amplitudes as in ordinary quantum mechanics. One can show that there is an underlying conceptual consistency: the extraction amplitude in the timeless framework reduces to this transition amplitude in the deparametrized framework [103].

Remarks.

(1) It has been suggested that, to obtain the correct extraction amplitude, one may need to sum over only those quantum geometries which have a positive time orientation [258]. However, it has been difficult to incorporate this condition in the current spin foam models [99–101]. Cosmological spin foams can be used to understand the difference from a physical perspective. The proposed condition is directly analogous to the LQC restriction to positive (or negative) frequency solutions to the constraints [103]. Without this condition, the inner product between physical states obtained by group averaging the basis elements $|v, \vec{l}, \phi\rangle$ would have been real, while the correct inner product coming from the Hamiltonian theory is complex. In the current spin foam models, the inner product between physical states defined by spin network states is also real. Thus, to the extent

cosmological spin foams provide hints for the full theory, it would appear that a restriction to time-oriented quantum histories is indeed necessary to complete the program.

(2) Most of the spin foam literature to date focuses on the vacuum case. On the other hand, the Bianchi I model considered in this section came with a scalar field [105]. In a timeless framework, a scalar field is unnecessary. What happens if we consider the vacuum Bianchi I model? In this case, although the extraction amplitude is again well defined in the Hamiltonian framework, if one mimics the Feynman procedure, the vertex expansion has to be regulated because it contains distributions term by term [104]. The analysis provides guidance on viable regulators that may be helpful more generally. However, one of its aspects is not entirely satisfactory: it is not possible to remove the regulator at the end of the day, whence the final answer still carries the memory of the specific regulator used. Thus, in this model, the inclusion of a matter field actually simplifies the vertex expansion. Perhaps there is a lesson here for the full theory.

(3) Because this section is devoted to lessons from LQC, we have focused on hints and suggestions that LQC has for the SFM and GFT programs. However, the bridge also goes the other way: in [106–108] proposals have been made to use SFM to go beyond homogeneous LQC. Although these proposals do not yet incorporate inhomogeneities of direct physical relevance, the underlying ideas are conceptually interesting.

7.4. Entropy bound and LQC

Bekenstein's seminal work [259] in which he suggested that the black hole entropy should be proportional to its area has motivated several researchers to ask if there is a geometrical upper bound on the maximum thermodynamic entropy that a system can have. The heuristic idea is as follows. The leading contribution to the black hole entropy is given by (1/4)th of the area of its horizon in Planck units. Since black holes are the 'densest' objects, one may be tempted to conjecture that in a complete quantum gravity theory, the number of states in any volume V enclosed by a surface of area A would be bounded by the number of states of a black hole with a horizon of area A, i.e. by $\exp A/4\ell_{\mathrm{Pl}}^2$. However, this simple formulation of the idea quickly runs into difficulties. Several improvements have been proposed. The most developed of these proposals is Bousso's covariant entropy bound [90]. The conjecture is as follows. Given a spatial 2-surface $\mathcal{B}$ with an area A, if $\mathcal{L}$ is the hypersurface generated by the non-expanding null geodesics orthogonal to $\mathcal{B}$, then the total entropy flux S across the 'light sheet' L (associated with matter) has an upper bound given by $S \leqslant A/4G\hbar$.

The conjecture has two curious features. First, it is not clear how to define the entropy flux without there being an entropy current s^a. If there is such a current, the flux across $\mathcal{L}$ can be defined as the integral of a 3-form: $S = \int_{\mathcal{L}} s^a \epsilon_{abcd}$ where ϵ_{abcd} is the volume 4-form. But 'fundamental' matter fields do not have an associated entropy current. Therefore, one can test the conjecture only for phenomenological matter such as fluids. Thus, there is tension between the notion that the bound should be fundamental and the domain in which it can be readily tested. The second curious feature is related to the fact that the bound makes a crucial use of the Planck length. Indeed, it trivializes if $\ell_{\mathrm{Pl}} \to 0$ and, as we show below, it is violated in classical general relativity. Yet, it also requires a smooth classical geometry so that light sheets can be well defined. Since quantum fluctuations are likely to make the spacetime geometry fuzzy, there is a tension between the classical formulation of the bound and the quantum world it is meant to capture.

In spite of these limitations, the bound does have a large domain of validity [91]: it holds if the entropy current and the stress–energy tensor satisfy certain inequalities on $\mathcal{L}$ and these inequalities can be motivated from statistical physics of ordinary matter so long as one stays

away from the Planck regime. Also the bound has attracted considerable attention because it has 'holographic flavor' and it has been suggested that 'holography' should be used as a building block of any quantum gravity theory, much as the equivalence principle was used in general relativity [260]. It is thus natural to ask what the status of the bound is in any putative quantum gravity theory. Specifically, there are two questions of interest. There are situations in which the bound fails in classical general relativity if applied in the Planck regime. The hope is that an appropriate quantum gravity treatment would restore it. The first question is: Does this happen? The second question is: Does the bound result only if the theory is constructed with a fundamental 'holographic' input or does it simply emerge in suitable regimes of the theory where it can be meaningfully formulated? It turns out that LQC is a near-ideal arena to address both these questions [89].

Let us consider a $k = 0$, $\Lambda = 0$ FLRW spacetime filled with a radiation fluid. The spacetime metric is given by

$$ds^2 = -dt^2 + a(t)^2 (dr^2 + r^2 \, d\Omega^2), \tag{7.16}$$

and choose the surface $\mathcal{B}$ to be a round 2-sphere in a homogeneous slice $t = $ const. The past-directed, ingoing null rays orthogonal to $\mathcal{B}$ provide us with its light sheet $\mathcal{L}$. Because the spacetime is conformally flat, these rays will all converge on a point p (in which case $\mathcal{L}$ would be the portion of the future light cone of p bounded by $\mathcal{B}$) or on the singularity. In what follows, we will consider only those $\mathcal{B}$ for which the first alternative occurs. Then, if we denote by t_f the time defined by $\mathcal{B}$ and t_i is the time defined by the point p, we have $t_i > 0$ and $A = 4\pi^2 a(t_f)^2 r_f^2$ where $r_f = \int_{t_i}^{t_f} dt'/a(t')$. For the null fluid, we have $p = 1/3\rho$ and, assuming that the universe is always instantaneously in equilibrium, by the Stefan–Boltzmann law, $\rho = (\pi^2/15\hbar^3)T^4$. The entropy current is therefore given by $s^a = (4/3)(\rho/T)u^a = (4\pi^2/45\hbar^3)T^3 u^a$, where u^a is the unit vector field orthogonal to the $t = $ const slices. Thus, the entropy current is completely determined by the temperature. Using the classical Friedman equation and the stress-energy conservation law, it is straightforward to obtain the temporal behavior of energy density, and therefore of temperature:

$$T(t) = \left(\frac{45\hbar^3}{32\pi^3 G t^2} \right)^{1/4}. \tag{7.17}$$

Therefore, if we were to move $\mathcal{B}$ to the past, the norm of the entropy current—and hence the flux of total entropy across its light sheet $\mathcal{L}$—would increase. A simple calculation gives [89]

$$\frac{S}{(A/4\ell_{\mathrm{Pl}}^2)} = \frac{2}{3} \left(\frac{2G\hbar}{45\pi t_f^2} \right)^{1/4} \left(1 - \sqrt{\frac{t_i}{t_f}} \right). \tag{7.18}$$

Note that $t_i/t_f < 1$ and as we move t_f closer to the singularity at $t = 0$, the right hand grows, just as one would expect from the behavior (7.17) of temperature. An explicit calculation shows that the right-hand side can exceed 1 by an arbitrary amount when t_f is so close to the singularity that $\rho \gtrsim 8.5\rho_{\mathrm{Pl}}$. Thus, in a radiation-filled FLRW universe, the bound can be violated by an arbitrary amount, but only in the Planck regime near the singularity. The question naturally arises: Do quantum gravity effects restore it?

As explained in the beginning of this subsection, it is not easy to analyze this issue because of the dual demand on the calculation: quantum gravity effects should be so strong as to resolve the singularity and at the same time one should be able to define space-like surfaces $\mathcal{B}$ *and* their light sheets $\mathcal{L}$ unambiguously. Fortunately, LQC meets this dual challenge successfully. As we have seen, non-perturbative LQG effects *are* strong enough to resolve the singularity and yet we have a smooth effective geometry which accurately tracks the quantum states of

interest across the big bounce. So the first question we began with can now be sharpened: Does the Bousso bound hold in the effective spacetime of LQC?

The analysis of entropy flux across $\mathcal{L}$ using the effective field equations can be carried out along the same lines as before. The modified Friedmann and Raychaudhuri equations again imply the standard continuity equation whence we again have $\rho \propto a^{-4}$. However, the modified Friedman and Raychaudhuri equations change the time dependence of the scale factor, energy density, and hence the temperature of the photon gas. The temperature now carries a dependence on the underlying quantum geometry via $\rho_{\max}$:

$$T(t) = \left(\frac{45\hbar^3}{32\pi^3 Gt^2 + \frac{3\pi^2}{\rho_{\max}}} \right)^{1/4}. \tag{7.19}$$

As one would expect, the temperature achieves its maximum value at the bounce, $t = 0$. But in stark contrast with the classical theory, it does not diverge. Therefore, the entropy current is also finite everywhere, including the bounce. As in the classical theory, one can compute the entropy current through $\mathcal{L}$ and obtain the desired ratio [89]

$$\frac{S}{(A/4\ell_{\rm Pl}^2)} = \frac{16}{9} \left(\frac{\pi^2 G^4 \hbar \rho_{\max}}{15} \right)^{1/4} \frac{1}{\sqrt{\frac{32\pi Gt_f^2}{3} + \frac{1}{\rho_{\max}}}} \left[t \; {}_2F_1 \left(\frac{1}{2}, \frac{1}{4}; \frac{3}{2}; -\frac{32\pi G\rho_{\max}}{3}t^2 \right) \right]_{t_i}^{t_f}, \tag{7.20}$$

where ${}_2F_1$ is a hypergeometric function which can be plotted numerically. From the fact that the temperature has an upper bound, it follows that the entropy current also has one and therefore we know analytically that the right-hand side is finite. But is it less than 1 as conjectured by Bousso? One finds $S/(4\ell_{\rm Pl}^2) < 0.976$ for all round $\mathcal{B}$! In retrospect, this is perhaps not all that surprising because even in general relativity the bound is violated only at densities $\rho \gtrsim 8.5\rho_{\rm PL}$ and in LQC we have $\rho \leqslant \rho_{\max} \approx 0.41\rho_{\rm Pl}$. But note that in LQC spacetime is extended and there are many more 'potentially dangerous' surfaces $\mathcal{B}$ in the Planck regime: one has to allow $\mathcal{B}$ whose light sheet $\mathcal{L}$ can meet and go past the $t = 0$ slice.

Thus, we have answered the first question: the quantum geometry effects of LQG do restore the Bousso bound for the round 2-spheres $\mathcal{B}$ in the radiation-filled FLRW universes. We can now turn to the second question: Is the bound fundamental? In this calculation, the fundamental ingredient was quantum geometry of LQG. That construction did not need anything like 'holography' as an input. Yet, the Bousso bound emerged in the effective theory where it could be properly formulated. Indeed, the conjecture cannot even be stated in full LQC where the geometry is represented by wavefunctions rather than smooth metrics. Thus, the analysis suggests that the covariant entropy bound–and its appropriate generalizations that may eventually encompass quantum field theory processes even on 'quantum corrected' but smooth spacetimes–can emerge from a fundamental quantum gravity theory in suitable regimes; they are not necessary *ingredients* in the construction of such a theory.

7.5. Consistent histories paradigm

Quantum theory is incomplete unless it includes a procedure to assign probabilities to events or histories. In open quantum systems, which allow an interaction with an environment or a classical external system, common ways to assign probabilities are the 'Copenhagen' interpretation and the environmental decoherence. However, for closed quantum systems, such as in quantum cosmology, these formulations are of little use. A quantum universe has neither an environment to enable a decoherence nor an external system inducing a collapse

of its wavefunction. Therefore, one needs a new strategy. A natural avenue is provided by the consistent histories approach that stems from the work of Hartle, Halliwell and others [109]. (See [25] for a detailed review and an extensive bibliography). This approach relies on computing a 'decoherence functional' between different histories and assigning consistent probabilities only to those histories whose interference vanishes. While the underlying ideas are very general, their application to full quantum gravity has, of necessity, remained rather formal. However, recently, this program has been carried out to completion to answer some key questions in the $k = 0$ WDW theory and sLQC. In the following, we first provide a brief summary of the paradigm and then sketch the analysis for the WDW theory following [110, 125]. The analysis for LQC has been performed in a similar fashion in [111].

The consistent histories approach uses three main inputs: (i) fine-grained histories, which constitute the most refined description of observables in a given time interval; (ii) coarse-grained histories, formed by dividing fine-grained histories in mutually exclusive sets governed by a specified range of eigenvalues of observables of interest, and (iii) a decoherence functional which is a measure of the interference between different branch wavefunctions corresponding to coarse-grained histories.

As an example, for a family of observables A^α (labeled by α) with eigenvalues $a_{k_i}^\alpha$ at time $t = t_i$, a coarse-grained history in which the eigenvalues fall in the range $\Delta a_{k_i}^\alpha$ in a time interval $t \in (t_1, t_n)$ is denoted by a class operator

$$
\begin{aligned}
C_h &= P_{\Delta a_{k_1}}^{\alpha_1}(t_1) P_{\Delta a_{k_2}}^{\alpha_2}(t_2) \cdots P_{\Delta a_{k_n}}^{\alpha_n}(t_n) \\
&= U(t_0 - t_1) P_{\Delta a_{k_1}}^{\alpha_1} U(t_1 - t_2) P_{\Delta a_{k_2}}^{\alpha_2} \cdots U(t_{n-1} - t_n) P_{\Delta a_{k_n}}^{\alpha_n} U(t_n - t_0).
\end{aligned} \tag{7.21}
$$

Here, $P_{\Delta a_{k_i}}^{\alpha_i}(t_i)$ denote Heisenberg projections at time t_i in the range $\Delta_{a_{k_i}}$, and $U(t)$ is the propagator defined by the Hamiltonian H. The branch wavefunction $|\Psi_h\rangle$ corresponding to the coarse-grained history h is determined by the action of the class operator: $|\Psi_h\rangle = C_h^\dagger |\Psi\rangle$. The interference between two coarse-grained histories is measured by the normalized decoherence functional: $d(h, h') = \langle \Psi_{h'}|\Psi_h \rangle$, which depends on the two histories h, h' as well as a pre-specified state Ψ. One can unambiguously assign probabilities to histories h and h' if the histories decohere, i.e. if $d(h, h') = 0$. In this case, the probability of the coarse-grained history h is given by $p(h) = d(h, h)$. In textbook quantum mechanics, one typically considers a single measurement. In this case, the class operator C_h is self-adjoint, the coarse-grained histories automatically decohere and one can assign probabilities unambiguously. In the more general context of multiple projectors, the class operator C_h is no longer self-adjoint and therefore histories do not automatically decohere. In this case, to assign probabilities, one has to first find coarse-grained histories that do.

Let us now turn to quantum cosmology and use this framework to calculate the probability for occurrence of singularities. Answering such questions, however, requires a reasonably good mathematical control on the quantum theory, in particular, knowledge of the physical inner product, families of observables and their properties and a notion of evolution and dynamics. Fortunately, these structures are now available in the WDW theory and sLQC of the $k = 0$ model coupled to a massless scalar field [76]. (The particular framework we will use in the WDW case is a direct spin-off of sLQC.) As we will discuss below, consistent histories analysis for WDW theory shows that the probability that a WDW quantum universe ever encounters a singularity is unity, independent of the choice of a state, even if arbitrary superpositions of expanding and contracting branches are allowed [110, 125]. By contrast, the analysis for sLQC shows that the probability for the universe to undergo a non-singular bounce is unity [111].

Let us consider the WDW theory. Following section 2.2, we can restrict our attention to (i) the positive frequency solutions of the quantum constraint (2.21); (ii) the scalar field

momentum $\hat{p}_{(\phi)}$, which is a constant of motion, and (iii) the relational observable $\hat{z}|_{\phi_o}$ which measures the logarithm of the physical volume of the universe at internal time ϕ_o. (For a treatment directly in terms of the volume $\hat{V}|_{\phi_o}$ itself, see [110, 125].) The propagator for the consistent histories framework is defined as

$$U(\phi - \phi_o) = e^{i\sqrt{\underline{\Theta}}(\phi - \phi_o)}. \tag{7.22}$$

We will be interested in coarse-grained histories in the range of eigenvalues Δz at internal time $\phi = \phi_o$. The corresponding projector consistent with the inner product (equation (2.23)) is trivially just

$$P_{\Delta z} = \int_{\Delta z} dz |z\rangle \langle z|. \tag{7.23}$$

Using the propagator and the projector, we can define the class operator corresponding to coarse-grained histories with logarithm of volume in the interval Δz :

$$C_{\Delta z|_{\phi^*}} = U^{\dagger}(\phi^* - \phi_o) P_{\Delta z}^z U(\phi^* - \phi_o) = P_{\Delta z}^z(\phi^*), \tag{7.24}$$

which leads to the branch wavefunction

$$|\Psi_{\Delta z|_{\phi^*}}(\phi)\rangle = U(\phi - \phi_o) C_{\Delta z|_{\phi^*}}^{\dagger} |\Psi\rangle. \tag{7.25}$$

The histories trivially decohere when the ranges of z have no overlap. Given a normalized state $\Psi(z, \phi)$, the probability for the universe to have a logarithm of volume in the range Δz at $\phi = \phi^*$ is given by the obvious expression

$$p_{\Delta z}(\phi^*) = \int_{\Delta z} dz |\Psi(z, \phi^*)|^2. \tag{7.26}$$

Thus, because so far we considerd just one measurement, the framework and the formulas are the familiar ones from ordinary quantum mechanics.

One can now pose questions about the probability for the occurrence of a singularity in the WDW theory. Since $\hat{p}_{(\phi)}$ is a constant of motion (and $\rho = p_{(\phi)}^2/2V^2$), one way to answer this question is by computing the probability for histories to enter an arbitrarily small interval of volume, i.e. an interval $\Delta z^\star = (-\infty, z^\star]$ in the logarithmic volume where $z^\star$ is an arbitrarily large negative number. Now, in the WDW theory, the right (contracting)- and the left (expanding)-moving modes belong to superselected sectors. Therefore, one can carry out the calculation separately in each sector, and find the probability for left-moving states to encounter the singularity in the distant past (and similarly, for the right-moving states in the distant future). For *arbitrary* left- and right-moving states (in the domains of operators under consideration), one obtains

$$\lim_{\phi \to -\infty} p_{\Delta z^\star}^L(\phi) = 1 \qquad \text{and} \qquad \lim_{\phi \to \infty} p_{\Delta z^\star}^R(\phi) = 1 \tag{7.27}$$

for any $z^\star$, however large and negative. Thus, the probability that an expanding WDW universe grows from an arbitrarily small volume turns out to be unity. Similarly, the probability that a contracting WDW universe enters an arbitrary small region of volume in the distant future is unity. In this calculation, limits $\phi \to \mp\infty$ are necessary because we are allowing *arbitrary* states. If one restricts the analysis to a semi-classical state which has a finite spread in volume, probability for the histories to enter $\Delta z^\star$ would become unit at a finite value of ϕ (which would depend on the state). The expectation value calculations in section 3.1 suggested this outcome. But that suggestion comes from intuition developed in quantum mechanics where the expectation values are tied to ensembles. The consistent histories analysis provides a precise statement for the single universe now under consideration. Note that because the decoherence between the mutually exclusive histories is exact (i.e. $d(h, h') = \delta_{h,h'}$), and the

probability is sharply 1, there is complete certainty that the singularity is not resolved in either the left- or the right-moving sector of the WDW theory.

So far, we considered left- and right-moving states independently and there may be concern that the certainty of our answer is a consequence of our not allowing superpositions. Indeed, for a superposed state $|\Psi\rangle = p_L|\Psi^L\rangle + p_R|\Psi^R\rangle$, with $p_L + p_R = 1$, the expectation value of the volume observable never vanishes. Naïvely, this could be taken as evidence that the universe described by this state avoids singularities. Furthermore, for this state,

$$\lim_{\phi \to -\infty} p_{\Delta z^\star}(\phi) = p_L \qquad \text{and} \qquad \lim_{\phi \to \infty} p_{\Delta z^\star}(\phi) = p_R, \tag{7.28}$$

whence one might conclude that there is a non-vanishing probability for a universe to have a large volume both in the asymptotic past and the future, i.e. for the universe to bounce in the WDW theory. How does this conclusion fare if we let go our intuition about expectation values that is rooted in ensembles and examine the issue in the consistent histories framework? Then, the conclusion turns out to be incorrect [110, 125]! We will now summarize why.

To analyze whether $\Psi = p_L|\Psi^L\rangle + p_R|\Psi^R\rangle$ represents a bouncing universe, it is necessary to compute the projections not just at one time slice, but at two time slices—one at a very early time and the other at a very late time—and ask: What is the probability of occurrence of any history that has large volume both in the distant past and in the distant future? Since the question refers to two instants of time, the required class operator is now more general than the ones considered in textbook quantum mechanics.

Let us begin by introducing the necessary ingredients. The class operator corresponding to a history in which the universe *does not* enter $\Delta z^\star$ at an early time ϕ_1 and a late time ϕ_2 is given by

$$C_{\text{large}}(\phi_1, \phi_2) = P^z_{(\Delta z_1^\star)_c}(\phi_1) P^z_{(\Delta z_2^\star)_c}(\phi_2), \tag{7.29}$$

where $(\Delta z^\star)_c$ is the complement of the interval $\Delta z^\star$. The coarse-grained history selected by this operator has volume larger than that represented by $z^\star$ at the two times considered. Therefore, in the limit at $\phi_1 \to -\infty$ and $\phi_2 \to \infty$, C_{large} can be interpreted as the class operator C_{bounce} representing bouncing histories. Similarly, the class operator representing a history that the universe does enter the interval $\Delta z^\star$ at both ϕ_1 and ϕ_2 is given by

$$C_{\text{small}}(\phi_1, \phi_2) = C_{\Delta z_1^\star} + C_{\Delta z_2^\star} - C_{\Delta z_1^\star; \Delta z_2^\star}. \tag{7.30}$$

Since the coarse-grained history selected by this operator has volume smaller than (or equal to) that represented by $z^\star$ at the two times considered, in the limit at $\phi_1 \to -\infty$ and $\phi_2 \to \infty$, C_{small} can be interpreted as the class operator C_{sing} representing histories that encounter singularities both in the future and the past.

One can show that the branch wavefunction for *any* superposed state $|\Psi\rangle = p_L|\Psi^L\rangle + p_R|\Psi^R\rangle$ to be in $(\Delta z^\star)_c$ both in the asymptotic past and the future is zero: $|\Psi_{\text{bounce}}\rangle = \lim_{\phi_1 \to -\infty} \lim_{\phi_2 \to \infty} C^\dagger_{\text{large}}(\phi_1, \phi_2)|\Psi\rangle = 0$. This shows that the probability associated with any bouncing coarse-grained history is identically zero. Similarly, the branch wavefunction corresponding to the history that is singular both in the asymptotic past and the asymptotic future turns out to be

$$|\Psi_{\text{sing}}\rangle = \lim_{\phi_1 \to -\infty} \lim_{\phi_2 \to \infty} C^\dagger_{\text{small}}(\phi_1, \phi_2)|\Psi\rangle = |\Psi\rangle \tag{7.31}$$

irrespective of how small the volume defined by $z^\star$ is. The decoherence functional between the histories which bounce and are singular vanishes identically. Therefore, it is meaningful to assign probabilities to these two coarse-grained histories. The probability that a universe is ever singular turns out to be unity. Thus, contrary to what one might have naïvely expected, arbitrary superpositions of contracting and expanding solutions do not avoid singularity in

the WDW theory. We emphasize that this result holds for any superposed state. Again, the prediction is completely unambiguous because the two coarse-grained histories decohere completely and because the associated probabilities are 1 and 0.

A similar calculation has been performed in sLQC [111]. It turns out that the probability that an arbitrary superposition of left- and right-moving states ever encounters a singularity is 0 and the probability for the bounce to occur is 1. Again, as in the WDW theory, these results bring out the precise sense in which the expectations based on results of section 3.1 are correct, without having to rely on the intuition derived from ensembles.

In summary, the consistent histories paradigm can be successfully realized for the $k = 0$ universes both in the WDW theory and LQC, thanks to the complete mathematical control on the quantum theory of these models. It provides precise answers to questions concerning probabilities of the occurrence of singularities in a quantum universe. This analysis provides a road map to use the consistent histories approach in more general contexts discussed in sections 3 and 6. These applications could lead to important insights on some long standing questions such as the quantum to classical transition in the cosmology of the early universe that is often evoked to account for the seeds of the large scale structure.

8. Discussion

The field of quantum cosmology was born out of the conviction that general relativity fails near the big-bang and the big-crunch singularities and quantum gravity will cure this blemish. In his 1967 lectures for Battelle Rencontres, John Wheeler wrote [32]:

> Here, according to classical general relativity, the dimensions of collapsing system are driven down to indefinitely small values.... In a finite proper time the calculated curvature rises to infinity. At this point the classical theory becomes incapable of further prediction. In actuality, classical predictions go wrong before this point. A prediction of infinity is not a prediction. The wave packet in superspace does not and cannot follow the classical history when the geometry becomes smaller in scale than the quantum mechanical spread of the wave packet.... The semiclassical treatment of propagation is appropriate in most of the domain of superspace.... [but] not so in the decisive region.

The quote is striking especially because of the certainty it expresses as to what should happen 'in actuality' near singularities. As we saw in sections 2–4, although this brilliant vision did not materialize in the WDW theory, it *is* realized in all the cosmological models that have been studied in detail in LQC. However, the mechanism is much deeper than just the 'finite width of the wave packet': the key lies in the quantum effects of geometry that descend from full LQG to the cosmological settings. These effects produce an unforeseen repulsive force. Away from the Planck regime the force is completely negligible. But it rises *very* quickly as curvature approaches the Planck scale, overwhelms the enormous gravitational attraction and causes the quantum bounce. Large repulsive forces of quantum origin are familiar in astrophysics. Indeed, it is the Fermi–Dirac repulsion between nucleons that prevents the gravitational collapse in neutron stars. Although this force is rooted in the purely quantum mechanical properties of matter, it is strong enough to balance classical gravitational attraction if the mass of the star is less than, say 5 solar masses. However, in heavier stars, classical gravity still wins and leads to black holes. In LQC the repulsive force has its origin in quantum geometry rather than quantum matter and it always overwhelms the classical gravitational attraction.

Thus, even though we began with just general relativity in four dimensions, quantum dynamics contains qualitatively new physics. This is a vivid illustration of the fact that higher dimensions or new symmetries are not *essential* for a quantum gravity theory to open new vistas. Indeed, a general lesson one can draw from LQG is that, even if a theory is firmly rooted in general relativity *in the classical domain*, its fundamental degrees of freedom can be far removed from what the classical continuum suggests. A coarse-grained description can suffice at low energies but the fundamental degrees of freedom become indispensable at the Planck scale. They can usher in new physics to overcome the ultraviolet difficulties of general relativity.

Sections 2–4 discussed three notable aspects of this physics beyond general relativity. First, although the exact solubility of the $k = 0$ FLRW model played a major role in establishing detailed analytical results [76] (such as the derivation of the expression of the maximum density ρ_{max}), systematic numerical studies have shown that the behavior in the Planck regime is much more general: the bounce persists in the FLRW models with spatial curvature or cosmological constant which are not exactly soluble [55, 56, 58]. More precisely, one can start with quantum states which are sharply peaked at late times on a general relativity trajectory and evolve them toward classical singularities. All wavefunctions that initially resemble coherent states undergo a quantum bounce at $\rho \approx \rho_{max}$ in the FLRW models and the behavior of these wavefunctions in the Planck regime is very similar. Since these models are not exactly soluble, one does not have results for general states. But the fact that there does exist a large class of physically interesting states exhibiting this behavior in the Planck regime is already highly non-trivial. Furthermore, in these models, there are now 'S-matrix-type' analytical results that relate the behavior of generic wavefunctions well before the bounce to that well after the bounce [145].[28]

The second notable feature is that this cure of the ultraviolet limitations of general relativity does *not* come at the cost of infrared problems. This is surprisingly difficult to achieve because, on the one hand, quantum dynamics has to unleash huge effects in the Planck regime and, on the other, it must ascertain that departures from general relativity at lower curvatures are so tiny that they do not accumulate over the immense cosmological time scales to produce measurable deviations at late times. Indeed, the early treatments of dynamics in LQC [37, 45] managed to resolve the singularity but, as we saw in section 7.1, gave rise to untenable deviations of general relativity at late times [52, 54]. To obtain good behavior in both the ultraviolet *and* the infrared requires a great deal of care and sufficient control on rather subtle conceptual and mathematical issues. The resulting 'improved dynamics' is now providing useful hints in full LQG [254]. Finally, it is pleasing to see that even in the models that are *not* exactly soluble, states that are semi-classical at a late initial time continue to remain sharply peaked throughout the low curvature domain. In the closed $k = 1$ model as well as $\Lambda < 0$ FLRW models, the universe undergoes a classical recollapse. For universes that grow to macroscopic sizes, predictions of LQC for this recollapse reduce to those of general relativity with impressive accuracy, thereby providing detailed quantitative tests of the good infrared behavior. Initially this is surprising because of one's experience with the spread of wavefunctions in non-relativistic quantum mechanics. However, this behavior is precisely

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[28] These advances required not only new conceptual ideas (e.g. relational time and specific Dirac observables) but a careful handling of difficult mathematical issues (such as essential self-adjointness of the gravitational constraints and control on their spectra) and the development of accurate numerical methods (that are attuned to the delicate mathematical properties of various operators). Because of our intended audience, in this review we focused on the conceptual issues and physical predictions and could not do justice to the seminal mathematical contributions, especially from the Warsaw group, nor to the powerful numerical infrastructure that was created almost singlehandedly by Tomasz Pawlowski.

what one would expect if at low curvature quantum gravity evolution is to agree with that in general relativity over cosmological time scales.

The third notable feature is the powerful role of effective equations [78–80] discussed in section 5. As is not uncommon in physics, their domain of validity is much larger than one might have naïvely expected from the assumptions that go into their derivations. Specifically, in all models in which detailed simulations of *quantum* evolution have been carried out, wavefunctions which resemble coherent states at late times follow the dynamical trajectories given by effective equations even in the deep Planck regime. These equations have two additional noteworthy features. First, they arise from a (first order) covariant action [199]. Second, although they introduce non-trivial corrections to *both* the Friedmann and the Raychaudhuri equations, the two modified equations continue to imply the correct equation of motion for matter (the Klein–Gordon equation for the scalar field and the continuity equation for a general perfect fluid). Thanks to all these features, there is growing confidence that the effective equations are likely to have a large domain of validity also in more complicated cosmological models. Therefore, even as a part of the LQC community is engaged in verifying their validity in, e.g., anisotropic models [166], others are actively engaged in working out their consequences, assuming they are valid more generally. These efforts have provided interesting insights. First, recall that cosmological singularities are not restricted to be of the big-bang or big-crunch type: even isotropic models which have perfect fluid matter (with an equation of state $P = P(\rho)$) admit a variety of more exotic singularities [173, 179]. Effective equations imply that all of the strong curvature singularities in isotropic and homogeneous models are resolved in LQC [173, 174]. Second, they have revealed the richness of the quantum bounces in more general models. In the isotropic case, there is a single bounce at which the scalar curvature and matter density reach their maxima. In the Bianchi models, the structure is much richer because of the non-triviality of Weyl curvature. Roughly, every time a shear term—a potential for the Weyl curvature—enters the Planck regime, the quantum geometry effects dilute them. Thus, in contrast to what was observed in other bouncing models, *anisotropies never diverge* in LQC [191]. This features removes a principal concern cosmologists have had [23]. Singularity resolution is both richer and more subtle in LQC because in anisotropic models there is not just one bounce; while there is still a 'density bounce' there are also 'bounces' associated with other observables such as the Weyl curvature.

This striking difference arises because the philosophy in LQC is different from the one implicitly used earlier in bouncing models. There, one first obtained a bounce in the FLRW model and then added other effects as corrections to the effective equations governing the bounce. In LQC, the philosophy is to first restrict oneself to an appropriate sector of the full phase space of general relativity with matter, pass to the corresponding truncated quantum gravity theory by applying principles of LQG, and finally distill effective equations from this quantum theory. Therefore, in the Planck regime, these equations can contain qualitatively new features, not seen in the FLRW model. This is exactly what happens in the anisotropic models discussed in sections 4.4 and 5.4. The very considerable research on the BKL conjecture [10, 11] in general relativity suggests that, as generic space-like singularities are approached, 'terms containing time derivatives in the dynamical equations dominate over those containing spatial derivatives' and dynamics of fields at any fixed spatial point is better and better described by the homogeneous Bianchi models. Therefore, to handle the Planck regime to an adequate approximation, it may well suffice to treat just the homogeneous modes using LQG and regard inhomogeneities as small deviations propagating on the resulting homogeneous LQC *quantum* geometries. This is the philosophy underlying 'hybrid quantization' which has successfully led to singularity resolution in the inhomogeneous Gowdy model [4–8]. However, an important

lesson from LQC is that it would not be adequate to treat just the isotropic degrees of freedom non-perturbatively and introduce anisotropies as small corrections.

Finally, in section 7, we discussed a few examples of fresh insights that LQC has provided into some of the long standing issues of quantum gravity, beyond cosmology. This is possible because the conceptual framework underlying LQC is well grounded and because there is an excellent mathematical control. An example is provided by the issue of entropy bounds [90, 91]: Should a suitable entropy bound constitute an essential ingredient in the very construction of a satisfactory quantum gravity theory, or would such bounds simply emerge from a quantum gravity theory on making suitable approximations in appropriate regimes? The issue is difficult to analyze because, while the bound has its origin in quantum gravity, its formulation requires a classical geometry. LQC provides an excellent setting to test these ideas because it can meet these stringent requirements. The detailed analysis [89] clearly favors the second possibility. Another example is provided by spin foams and group field theory. Here, LQC could be used to test general ideas underlying these paradigms. Specifically, does the 'extraction amplitude'—that replaces the more familiar 'transition amplitude' in the timeless quantum gravity framework—admit a meaningful 'vertex expansion' in line with the goals of these framework? Since the Hamiltonian theory underlying LQC is fully under control, this and other more detailed questions could be explored in detail in LQC. The calculations not only provide a strong support for the paradigm but also raise specific questions for further work [102–105].

A third example is provided by the application of the consistent histories framework. In full quantum gravity, of necessity, the application has only been formal. LQC provides a well-controlled setting which has all the major conceptual difficulties of full quantum gravity that require a generalization of the standard 'Copenhagen' quantum mechanics [24–28]. The fact that this framework can be used to address in detail concrete questions of physical interest in quantum cosmology [110, 125] opens doors for more general applications. Next, there is a recent proposal to construct LQG for general relativity coupled with massless scalar fields [92] that draws on strategies used in LQC: the use of a scalar field as relational time, construction of the physical Hilbert space from 'positive frequency' solutions to the quantum constraints and introduction of Dirac observables analogous to the $\hat{V}|_\phi$, $\hat{p}_\phi$ in LQC. In all these examples, LQC provided conceptual and mathematical tools to address in a concrete fashion some of the issues we face in full quantum gravity. The last example also represents progress in the other direction. So far there are only a few partial results on the precise relation between full LQG and LQC [261, 262]. If the proposal of [92] can be shown to be physically viable, it would provide a natural avenue to systematically descend from LQG to LQC. Finally, in light of the BKL conjecture [10, 11] and its recent formulation adapted to the LQG phase space [263], the LQC singularity resolution in Bianchi models [3, 61, 62] opens up an avenue to study the fate of general space-like singularities in quantum gravity. Specifically, one can now hope to prove theorems in support of the idea that strong curvature, space-like singularities are absent in LQG.

Returning to the more restricted setting of cosmology, it seems fair to say that LQC provides a coherent and conceptually complete paradigm that is free from the difficulties associated with the big bang and the big crunch. Therefore, the field is now sufficiently mature to address observational issues. Indeed, this is the most fertile and interesting of directions for current and future research. Not surprisingly, then, it has begun to attract the attention of main-stream cosmologists (see, e.g., [70–75, 188, 193, 197, 203, 205, 207, 239, 247, 249, 264, 265]).

There is already significant literature that has begun to probe in detail how the novel effects associated with LQC—the quantum bounce, the superinflation phase and the holonomy and the

inverse volume corrections—can affect the current cosmological scenarios based on general relativity. Much of this work—*though not all*—is based on inflationary scenarios. On the conceptual side, because the big-bang singularity is replaced by the quantum bounce where all fields are regular, one can resolve the difficulties associated with measures on spaces of solutions and carry out a well-defined calculation of the *a priori* probability of inflation. A pleasant surprise was that the probability turned out to be extremely close to one in spite of the non-trivialities of dynamics associated with superinflation and the phase that immediately follows it [82, 83]. On the phenomenological side, it is heartening to see detailed calculations on possible modifications of spectral indices and close connection to WMAP observations. Because this literature is still evolving, we do not yet have definitive predictions on which there is general consensus. Therefore, in section 6.4 we only provided illustrative examples. A significant fraction of this work is devoted to the inflationary and post-inflation phases. Although these quantum gravity corrections are conceptually interesting, since the curvature and matter densities at the onset of inflation are some 11 orders of magnitude smaller than the Planck scale, these effects will not be observable in the foreseeable future. Effects that could be relevant for such observations will have to originate in the deep Planck regime and not dilute away during inflation. As discussed in section 6.3, there are some viable possibilities along these lines and a systematic framework—involving quantum fields (representing linear perturbations) on quantum (FLRW) spacetimes—necessary to exploit them has become available. Therefore, there is much scope for synergistic work from cosmology and LQG communities in this growing area.

We hope this review will help to attract a broader participation from the cosmology community to achieve this goal.

Acknowledgments

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