General Relativity and Gravitation (2011)
DOI 10.1007/s10714-009-0763-4

REVIEW ARTICLE

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Loop quantum cosmology: an overview

Received: 30 November 2008 / Accepted: 17 December 2008

Abstract A brief overview of loop quantum cosmology of homogeneous isotropic models is presented with emphasis on the origin of and subtleties associated with the resolution of big bang and big crunch singularities. These results bear out the remarkable intuition that John Wheeler had. Discussion is organized at two levels. The the main text provides a bird's eye view of the subject that should be accessible to non-experts. Appendices address conceptual and technical issues that are often raised by experts in loop quantum gravity and string theory.

Keywords Loop quantum cosmology, Singularity resolution, Planck scale physics, Quantum geometry

1 Introduction

In general relativity, the gravitational field is encoded in the very geometry of space–time. Geometry is no longer an inert backdrop providing just a stage for physical happenings; it is a physical entity that interacts with matter. As we all know, this deep paradigm shift lies at the heart of the most profound predictions of the theory: the big bang, the black holes and the gravitational waves. However, the encoding of gravity in geometry also implies that space–time itself must end when the gravitational field becomes singular, and *all of physics* must come to an abrupt halt. This is why in popular articles relativists and cosmologists like to say that the universe was born with a big bang some 14 billion years ago and it is meaningless to ask what was there before. In more technical articles they point out that this finite beginning leads to the 'horizon problem.' But we know that general relativity is incomplete because it ignores quantum physics. If we go back in time using general relativity, we encounter huge matter densities and curvatures

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at which quantum effects should in fact dominate physics. This is the regime where we can no longer trust general relativity. *Thus, the big bang is a prediction of general relativity precisely in a domain where it is inapplicable.* Although in the framework of general relativity the universe did begin with a big-bang, there is no reason to believe that the real, physical universe did.

To know what really happened, one needs a quantum theory of gravity. John Wheeler recognized this early and drew on various analogies to argue that quantum fluctuations of geometry would intervene and resolve classical singularities. Already in his 1967 lectures in Battelle Rencontres, he wrote [1]:

> *In all applications of quantum geometrodynamics, none would seem more immediate than gravitational collapse 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 of interest to gravitational collapse. Not so in the decisive region.*

Wheeler focused on the gravitational collapse but his comments are equally applicable to the big-bang—the time reverse of the collapse. This point was made explicit is Misner's articles on quantum cosmology [2], particularly in his contribution to the Wheeler Festschrift.

However, It turned out that within the framework of quantum geometrodynamics (QGD) that Wheeler, Misner and DeWitt used, without additional inputs the big bang singularity could not be resolved generically, at least in the precise, physical sense spelled out in Sect. 4. The subject had therefore remained rather dormant for over two decades. Over the last 6–7 years, the issue was revived in the context of loop quantum cosmology (LQC) [3; 4]—the application of loop quantum gravity (LQG) [5; 6; 7] to cosmological models. The LQG program is rather similar to that envisaged by Wheeler: both are canonical approaches, both follow pioneering ideas of Bergmann and Dirac, and in both cases dynamics has to be teased out of the quantum Hamiltonian constraint. There is however, a key difference: LQG is based on a specific quantum theory of Riemannian geometry. As a result, geometric observables display a fundamental discreteness [8; 9; 10; 11]. It turns out that this discreteness plays a key role in quantum dynamics: While predictions of LQC are very close to those of QGD away from the Planck regime, there is a dramatic difference once densities and curvatures enter the Planck scale. In LQC the big bang is replaced by a quantum bounce. Moreover, thanks to the introduction of new analytical and numerical methods over the past two years, it is now possible to probe the Planck scale physics in detail.

The purpose of this article is to present an overview of the situation. Since the intended audience is diverse, I will present the material at two levels. In the main body, I will summarize the main developments, emphasizing the conceptual aspects[1] from an angle that, I hope, will make the material accessible also to non-experts. In the Appendices, I will address a number of more technical issues that are often raised in LQG as well as string theory circles.

The material is organized as follows. In Sect. 2 I will set the stage by listing some key questions on the nature of the big bang that any quantum theory of gravity should address. In Sect. 3, I will summarize the situation in the Wheeler DeWitt theory. Because LQC has evolved considerably since its inception, the cumulative discussion in the literature can seem somewhat confusing to non-experts. Therefore, I will begin in Sect. 4 by outlining this evolution of the subject and then explain the key difference between LQC and QGD (also known as the Wheeler-DeWitt (WDW) theory). Main results of LQC are gathered in Sect. 5. Section 6 summarizes the overall situation from a broad perspective. Appendix A discusses some conceptual issues and B, issues related to dynamics.

2 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 and Wheeler. More recent developments in inflationary and cyclic models raise additional issues. In this section, I will present a prototype list. It is far from being complete but should suffice to provide an approach independent gauge to compare the status of various programs.

- How close to the big-bang does a smooth space–time of general relativity make sense? Inflationary scenarios, for example, are based on a space–time 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? As we saw in Sect. 1, this tantalizing possibility 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 [12]. 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 deterministic evolution? The idea that there was a pre-big-bang branch to our universe has been advocated in

[1] Thus I will not include any derivations but instead provide references where the details can be found.

several approaches, most notably by the pre-big-bang scenario in string theory [13] and ekpyrotic and cyclic models [14; 15] inspired by the brane world ideas. However, these are perturbative treatments which require a smooth continuum in the background. Therefore, their dynamical equations break down at the singularity whence, without additional input, the pre-big-bang branch is not joined to the current post-big-bang branch by a deterministic evolution. 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?

Clearly, to answer such questions we cannot start by assuming that there is a smooth space–time 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 space–time. In quantum gravity, this issue becomes even more vexing.[2]

For simple systems, including Minkowskian field theories, the Hamiltonian formulation generally serves as the royal road to quantum theory. It was therefore adopted for quantum gravity by Dirac, Bergmann, Wheeler and others. But absence of a background metric implies that the Hamiltonian dynamics is generated by constraints [17; 18]. 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 wave function, 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 [19]. 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, emphasized by Green and Unruh [20] in the context of an older LQC treatment of the $k = 1$ model:

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

[2] There is a significant body of literature on issue; see, e.g., [16] and references therein. These difficulties are now being discussed also in the string theory literature in the context of the AdS/CFT conjecture.

Fig. 1 **a** Classical solutions in $k = 0$, $\Lambda = 0$ FRW models with a massless scalar field. Since $p_{(\phi)}$ is a constant of motion, a classical trajectory can be plotted in the v–ϕ plane, where v is the volume (essentially in Planck units) of a fixed fiducial cell. 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. **b** Classical solutions in the $k = 1$, $\Lambda = 0$ FRW model with a massless scalar field. The universe begins with a big bang, expands to a maximum volume and then undergoes a recollapse to a big crunch singularity. Since the volume of the universe is double valued in any solution, it cannot serve as a global time coordinate in this case. The scalar field on the other hand does so both in the $k = 0$ and $k = 1$ cases

By their very construction, perturbative and effective descriptions have no problem with the second requirement. However, physically their implications can not be trusted at the Planck scale and mathematically they generally fail to provide a deterministic evolution across the putative singularity. Since the non-perturbative approaches often start from deeper ideas, it is conceivable that they could lead to new structures at the Planck scale which modify the classical dynamics and resolve the big-bang singularity. 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} gms/cc 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!

The question then is: How do various approaches fare with respect to these questions? In LQC these issues have been addressed in considerable detail. As we will see in Sects. 4 and 5, some of them could be addressed even in the simplest, early versions of the theory, while others required a much more careful analysis of the quantum Hamiltonian constraint.

3 FRW models and the WDW theory

Almost all phenomenological work in cosmology is based on the $k = 0$ homogeneous and isotropic Friedmann Robertson Walker (FRW) space–times and perturbations thereof. Therefore, these models provide a natural point of departure for quantum cosmology. For concreteness, I will focus on FRW model in which the only matter source is a massless scalar field (although our discussion will make it clear that it is relatively straightforward to allow additional fields, possibly with complicated potentials). I will consider $k = 0$ (or spatially flat) as well as $k = 1$ (spatially closed) models. Conceptually, these models are interesting for our purpose because *every* of their classical solutions has a singularity (see Fig. 1). Therefore a natural singularity resolution without external inputs is highly non-trivial. In light of the spectacular observational inputs over the past decade, the $k = 0$ model is the one that is phenomenologically most relevant. However as we will see, because of its classical recollapse, the $k = 1$ model offers a more stringent viability test for the quantum cosmology.

Let us begin with the issue of time. In the classical theory, one considers one space–time at a time and although the metric of that space–time is dynamical, it enables one to introduce time coordinates—such as the proper time—that have direct physical significance. However in the quantum theory—and indeed already in the phase space framework that serves as the stepping stone to quantum theory—we have to consider all possible homogeneous, isotropic space–times. In this setting one can introduce a natural foliation of the 4-manifold, each leaf of which serves as the 'home' to a spatially homogeneous 3-geometry. However, unlike in non-gravitational theories, there is no preferred physical *time variable* to define evolution. As discussed in Sect. 2, a natural strategy is to use part of the system as an 'internal' clock with respect to which the rest of the system evolves. This leads one to Leibnitz's *relational time*. Now, in any spatially homogeneous model with a massless scalar field ϕ, the conjugate momentum $p_{(\phi)}$ is a constant of motion, whence ϕ is monotonic along any dynamical trajectory. Thus, in the classical theory, it serves as a global clock[3] (see Fig. 1). Questions about evolution can thus be phrased as: 'If the curvature or matter density or an anisotropy parameter is such and such when $\phi = \phi_1$ what is it when $\phi = \phi_2$?'

What is the situation in the quantum theory? There is no a priori guarantee that a variable which serves as a viable time parameter in the classical theory will continue to do so in the quantum theory. Whether it does so depends on the form of the Hamiltonian constraint. For instance as Fig. 1a shows, in the $k = 0$ model without a cosmological constant, volume (or the scale factor) can be used as a global 'clock' along any classical trajectory. But the form of the quantum Hamiltonian constraint [21] in LQG is such that it does not readily serve this role in the quantum theory. The scalar field ϕ, on the other hand, continues to do so (with or without a cosmological constant and also in the $k = 1$ case).[4]

Let us now turn to quantization. Because of the assumption of spatial homogeneity, we have only a finite number of degrees of freedom. Therefore, although the conceptual problems of quantum gravity remain, there are no field theoretical infinities and one can hope to mimic ordinary text book quantum mechanics to pass to quantum theory. However, in the $k = 0$ case, because space is infinite, homogeneity implies that the action, the symplectic structure and Hamiltonians all diverge since they are represented as integrals over all of space. Therefore, in any approach to quantum cosmology—irrespective of whether it is based on path integrals or canonical methods—one has to introduce an elementary cell $\mathscr{C}$ and restrict all integrals to it. In actual calculations, it is generally convenient also

[3] Although ϕ is a good evolution parameter, it does not have physical dimensions of time. Still in what follows we will loosely refer to it as 'time' for simplicity.

[4] As I mentioned in Sect. 2, while the availability of an internal evolution parameter such as ϕ makes it easier to interpret the theory, a preferred time variable,—especially one that is defined globally—is not essential. If there is no massless scalar field, one could still use a suitable matter field as a 'local' internal clock. For instance, in the inflationary scenario, because of the presence of the potential, the inflation is not monotonic even along classical trajectories. But it is possible to divide dynamics into 'epochs' and use the inflation as a clock locally, i.e., within each epoch [22]. There is considerable literature on the issue of internal time for model constrained systems [16] (such as a system of two harmonic oscillators where the total energy is constrained to be constant [23]).

to introduce a fiducial 3-metric ${}^o q_{ab}$ (as well as frames ${}^o e_i^a$ adapted to the spatial isometries) and represent the physical metric q_{ab} via a scale factor a, $q_{ab} = a^2\, {}^o q_{ab}$. Then the geometrical dynamical variable can be taken to be either the scale factor a or the 'oriented' volume v of the fiducial cell $\mathscr{C}$ as measured by the physical frame e_i^a, where v is positive if e_i^a has the same orientation as ${}^o e_i^a$ and negative if the orientations are opposite. (In either case the physical volume of the cell is $|v|$.) In LQC it is more convenient to use v rather than the scale factor so we will use v here as well. Note, however, that physical results cannot depend on the choice of the fiducial cell $\mathscr{C}$ or the fiducial metric ${}^o q_{ab}$.[5] In the $k = 1$ case, since space is compact, a fiducial cell is unnecessary and the dynamical variable v is then just the oriented physical volume of the universe.

With this caveat about the elementary cell out of the way, one can proceed with quantization. Situation in the WDW theory can be summarized as follows. This theory emerged in the late sixties and was analyzed extensively over the next decade and a half [17; 18]. Many of the key physical ideas of quantum cosmology were introduced during this period [2; 19] and a number of models were analyzed. However, since a mathematically coherent approach to quantization of full general relativity did not exist, there were no guiding principles for the analysis of these simpler, symmetry reduced systems. Rather, quantization was carried out following 'obvious' methods from ordinary quantum mechanics. Thus, in quantum kinematics, states were represented by square integrable wave functions $\Psi(v,\phi)$, where v represents geometry and ϕ, matter; and operators $\hat{v}, \hat{\phi}$ acted by multiplication and their conjugate momenta by ($-i\hbar$ times) differentiation.

Because of spatial homogeneity and isotropy, we are left with a single Hamiltonian constraint; all others are automatically solved. The Hamiltonian constraint takes the form of a differential equation that must be satisfied by the physical states [24]:

$$\partial_\phi^2 \underline{\Psi}(v,\phi) = \underline{\Theta}_o \underline{\Psi}(v,\phi) := -12\pi G\,(v\partial_v)^2\, \underline{\Psi}(v,\phi) \tag{3.1}$$

for $k = 0$, and

$$\partial_\phi^2 \underline{\Psi}(v,\phi) = -\underline{\Theta}_1 \underline{\Psi}(v,\phi) := -\underline{\Theta}_o \underline{\Psi}(v,\phi) - GC\,|v|^{\frac{4}{3}}\, \underline{\Psi}(v,\phi), \tag{3.2}$$

for $k = 1$, where C is a numerical constant. (The bars below various symbols indicate that they refer to the WDW theory.) *In what follows* $\underline{\Theta}$ *will stand for either* $\underline{\Theta}_o$ *or* $\underline{\Theta}_1$. These are the celebrated WDW equations of the two models. In the older literature, the emphasis was on finding and interpreting the WKB solutions of these equations (see, e.g., [25]). However, as Wheeler emphasized already in 1968 [1], the WKB approximation fails near the singularity and we need an exact quantum theory.

The physical sector of the WDW theory can be readily constructed [21; 24]. A systematic procedure based on the so-called group averaging method [26; 27; 28] (which is applicable for a very large class of constrained systems) provides the physical inner product on the space of solutions $\underline{\Psi}(v,\phi)$ to the WDW equation. To understand its structure, note that the form of (3.1) and (3.2) is the same as

[5] This may appear as an obvious requirement but unfortunately it is often overlooked in the literature. The claimed physical results often depend on the choice of $\mathscr{C}$ and/or ${}^o q_{ab}$ although the dependence is often hidden by setting the volume v_o of $\mathscr{C}$ with respect to ${}^o q_{ab}$ to 1 (in unspecified units) in the classical theory.

that of a Klein–Gordon equation in a 2-dimensional static space–time (with a ϕ-independent potential in the $k = 1$ case), where ϕ plays the role of time and v of space. This suggests that we think of ϕ as the relational time variable with respect to which v, the 'true' degree of freedom, evolves. Not surprisingly, the scalar product given by the group averaging procedure coincides with the expression from the Klein–Gordon theory in static space–times.

The resulting physical sector of the final theory can be summarized as follows. The physical Hilbert space $\mathscr{H}_{\text{phy}}$ in the $k = 0$ and $k = 1$ cases consists of 'positive frequency' solutions to (3.1) and (3.2) respectively. A complete set of observables is provided by the momentum $\hat{p}_{(\phi)}$ and the relational observable $\hat{|v|}|_{\phi_o}$ representing the volume at the 'instant of time ϕ_o':

$$\hat{p}_{(\phi)}\,\underline{\Psi}(v,\phi) = -i\hbar\partial_\phi\,\underline{\Psi}(v,\phi)$$
$$\text{and}\quad \hat{V}|_{\phi_o}\,\underline{\Psi}(v,\phi) = e^{i\sqrt{\Theta}(\phi-\phi_o)}\,|v|\,\Psi(v,\phi_o). \tag{3.3}$$

(Thus, the action of $\hat{|v|}|_{\phi_o}$ is as follows: One freezes the given solution to the WDW equation at 'time' ϕ_o, acts of the volume operator and then evolves the new initial data to obtain another solution.) There are *Dirac* observables because their action preserves the space of solutions to the constraints and are self-adjoint on the physical Hilbert space $\mathscr{H}_{\text{phy}}$. With this exact quantum theory at hand, we can ask if the singularities are naturally resolved.

More precisely, from $\hat{p}_{(\phi)}$ and $\hat{V}|_\phi$ we can construct observables corresponding to matter density $\hat{\rho}$ (or space–time scalar curvature $\hat{R}$). Since the singularity is characterized by divergence of these quantities in the classical theory, in the quantum theory we can proceed as follows. We can select a point (v_o,ϕ_o) at a 'late time' ϕ_o on a classical trajectory of Fig. 1—e.g., the present epoch in the history of our universe—when the density and curvature are *very* low compared to the Planck scale, and construct a semi-classical state which is sharply peaked at v_o at $\phi = \phi_o$. We can then evolve this state *backward* in time. Does it follow the classical trajectory? To have the correct 'infra-red' behavior, it must, until the density and curvature become very high. What happens in this 'ultra-violet' regime? Does the quantum state remain semi-classical and follow the classical trajectory into the big bang? Or, does it spread out making quantum fluctuations so large that although the quantum evolution does not break down, there is no reasonable notion of classical geometry? Or, does it remain peaked on some trajectory which however is so different from the classical one that, in this backward evolution, the universe 'bounces' rather than being crushed into the singularity? Or, does it... Each of these scenarios provides a distinct prediction for the ultra-violet behavior and therefore for physics in the deep Planck regime.[6]

[6] Sometimes apparently weaker notions of singularity resolution are discussed. Consider two examples [29]. One may be able to show that the wave function vanishes at points of the classically singular regions of the configuration space. However, the *physical* inner product could well be non-local in this configuration space, whence such a behavior of the wave function would not imply that the probability of finding the universe at these configurations is zero. The second example is that the wave function may become highly non-classical. This by itself would not mean that the singularity is avoided unless one can show that the expectation values of a family of Dirac observables which become classically singular remain finite there.

Fig. 2 Expectation values (and dispersions) of $|\hat{v}|_\phi$ for the WDW wave function in the $k = 1$ model. The WDW wave function follows the classical trajectory into the big-bang and big-crunch singularities ($p_{(\phi)}$ is a constant of motion. In this simulation, the quantum state at late times is a Gaussian peaked at $p_{(\phi)} = 5000\hbar$ in the $G = c = 1$ units and the dispersion is $\Delta p_{(\phi)}/p_{(\phi)} = 0.02$)

It turns out that the WDW theory leads to similar predictions in both $k = 0$ and $k = 1$ cases [21; 24; 30; 31]. They pass the infra-red tests with flying colors (see Fig. 2). But unfortunately the state follows the classical trajectory into the big bang (and in the $k = 1$ case also the big crunch) singularity. Thus the first of the possibilities listed above is realized. The singularity is not resolved because expectation values of density and curvature continue to diverge in epochs when their classical counterparts do. The analogy to the hydrogen atom discussed in Sect. 2 fails to be realized in the WDW theory of these simple models.

4 LQC: preliminaries

For a number of years, the failure of the WDW theory to naturally resolve the big bang singularity was taken to mean that quantum cosmology cannot, by itself, shed significant light on the quantum nature of the big bang. Indeed, for systems with a finite number of degrees of freedom we have the von Neumann uniqueness theorem which guarantees that quantum kinematics is unique. The only freedom we have is in factor ordering and this was deemed insufficient to alter the status-quo provided by the WDW theory.

The situation changed dramatically in LQG. In contrast to the WDW theory, a well established, rigorous kinematical framework *is* available in full LQG [5; 6; 7; 8]. 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 a natural resolution of the big bang singularity.

These developments occurred in three stages, each of which involved major steps that overcame limitations of the previous one. As a consequence, the viewpoint and the level of technical discussions has evolved quite a bit. Therefore many statements made in the literature have become outdated. Since non-experts can be confused by the occasional tension between statements made at different stages of this evolution, I will now make a small detour to summarize how the subject evolved.

4.1 Development of the subject

The first seminal contribution was Bojowald's result [32] that the quantum Hamiltonian constraint of LQC does not break down at $a = 0$ where the classical singularity occurs. Since this was a major shift that overcame the perceived impasse suggested by the WDW theory, it naturally led to a flurry of activity and the subject began to develop. 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 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 key input from Klaus Fredenhagen at the same workshop, it was soon realized [33] that in cosmological models one can mimic the procedure used in full LQG to remove the periodicity assumption. In the full theory, the requirement of diffeomorphism covariance leads one to a *unique* representation of the algebra of fundamental operators [34; 35]. If one mimics in LQC the procedure followed in the full theory, one finds K naturally takes values on the real line as one would want physically. But as I mentioned above, the resulting quantum kinematics is *inequivalent* to that of the WDW theory and the quantum Hamiltonian constraint is now a regular operator without having to assume 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 [33] 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, none of the analyses had a physical Hilbert space nor well-defined Dirac observables. Indeed, often the Hamiltonian constraint failed to be self-adjoint on the kinematical Hilbert space whence one could not even begin to use the group averaging method. Consequently, new questions arose. In particular, Brunnemann and Thiemann [36] 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 internal 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, 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 this issue [21; 24; 37]. The physical Hilbert space could again be constructed using the massless scalar field ϕ as internal time. It was found [21] that the self-adjoint version of the Hamiltonian constraint introduced in the second stage [33]—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 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 [24], and [38].) First, the matter density (or curvature scalar) at which the bounce occurs depended sensitively on quantum states and, unfortunately, more semiclassical the state, lower was the density at which the bounce occurred. Therefore the theory predicted huge deviations from general relativity even at the density of water! Second, when cosmological constant is non-zero, large deviations from general relativity can occur even at late times, i.e., *well away* from the Planck regime. This is a concrete manifestation of the ultraviolet-infrared tension discussed in Sect. 2. Finally, this quantum dynamics has a deep conceptual flaw: in the $k = 0$ model, even the leading order predictions depend on the choice of the fiducial cell, an auxiliary structure which has no physical significance. This meant that, in spite of the singularity resolution, the theory was physically unacceptable.

Fortunately, the problem could be traced back to the fact that quantization [21; 33] of the Hamiltonian constraint had ignored a conceptual subtlety. Roughly, at a key step in the procedure, the Hamiltonian constraint operator of [33] implicitly used the kinematic metric q^o_{ab} rather than the physical metric q_{ab}. When this is corrected, the new, improved Hamiltonian constraint again *resolves the singularity and, at the same time, is free from all the drawbacks of the* μ_o *scheme*. This is one of the best examples of the deep interplay between physics and mathematics that I have encountered. 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 (see Sect. 4.2). $\bar{\mu}$ dynamics has been successfully implemented in the case of a non-zero cosmological constant [24; 39; 40], the $k = 1$, spatially compact case [30; 31], and to the Bianchi I model [41]. As I mentioned earlier, in the $k = 1$ model, Green and Unruh [20] 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 from a mathematical physics perspective [31; 42; 43]. This work uses a combination of analytic and numerical techniques to enhance rigor to a level that is unprecedented in quantum cosmology.

We are now in the fourth stage of LQC where two directions are being pursued. In the first, emphasis is on extending the framework to more and more general situations (see in particular [22; 44]). 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. The analysis of Bianchi I models has re-enforced my belief that this lesson is an extremely valuable guide for generalizations. It narrows down choices by making direct appeal to physical considerations. The second direction in current work is LQC phenomenology. Various LQC effects are being incorporated in the analysis of observed properties of CMB particularly by cosmologists (see, e.g., [45; 46; 47; 48; 49; 50]). These investigations explore a wide range of issues, including: (i) effects of the quantum-geometry driven super-inflation just after the big-bounce, predicted by LQC; (ii) LQC driven effects on dark energy and phantom fields; and, (iii) production of gravitational waves near the big bounce. They combine very diverse ideas and are therefore important. However, since most of this analysis has been carried out by cosmologists who are not experts in quantum gravity, it does not always do justice to all the relevant features, predictions and subtleties of LQC. This frontier is still to mature. But the body of work that has accumulated so far does provide an excellent scaffolding and LQC community has begun to use it to build a more careful, reliable and detailed framework.

4.2 New quantum mechanics

Let us return to the difference between the WDW theory and LQC. As I mentioned at the beginning of Sect. 4, in the eighties and nineties von-Neumann's uniqueness theorem and results from the WDW theory had led to a general belief that the big bang singularity can not be resolved in quantum cosmology. So what happens to the von Neumann theorem in LQC?

Let us first recall the statement of the theorem: 1-parameter groups $U(\lambda)$ and $V(\mu)$ satisfying the Weyl commutation relations[7] admit (up to isomorphism) a unique irreducible representation by unitary operators on a Hilbert space $\mathscr{H}$ in which $U(\lambda)$ and $V(\mu)$ are weakly continuous in the parameters λ and μ. By Stone's theorem, weak continuity is a necessary and sufficient condition for $\mathscr{H}$ to admit self adjoint operators $\hat{x}, \hat{p}$ such that $U(\lambda) = e^{i\lambda\hat{x}}$ and $V(\mu) = e^{i\mu\hat{p}}$. Therefore assumption of the von Neumann theorem are natural in non-relativistic quantum mechanics and we are led to a unique quantum kinematics—the Schrödinger theory.

However, in full LQG, x is analogous to the gravitational connection and $U(\lambda)$ to its holonomy. One can again construct an abstract algebra using holonomies and operators conjugate to connections and ask for its representations satisfying natural assumptions, the most important of which is the diffeomorphism covariance dictated by background independence. There is again a uniqueness theorem [34; 35]. However, in the representation that is thus singled out, holonomy operators—analogs of $U(\lambda)$—*fail to be weakly continuous* whence there are no operators corresponding to connections! Furthermore, a number of key features of the theory—such as the emergence of a quantum Riemannian geometry in which there is fundamental discreteness—can be traced back to this unforeseen feature. Therefore, upon symmetry reduction, although we have a finite number of degrees of freedom, it would be incorrect to just mimic Schrödinger quantum mechanics and impose weak continuity. When this assumption is dropped, the von Neumann theorem is no longer applicable and *we can have new quantum mechanics* [33]. This new kinematical arena is constructed by applying the procedure used in full LQG to the symmetry reduced models of LQC.

Thus, the key difference between LQC and the WDW theory lies in the fact that while one does not have reliable quantum kinematics in the WDW theory, there is a well developed and rigorous framework in LQG which, furthermore, is *unique*! If we mimic it as closely as possible in the symmetry reduced theories, we are led to a new kinematic arena, distinct from the one used in the WDW quantum cosmology. LQC is based on this arena.

5 LQC: dynamics

It turns out WDW dynamics is not supported by the new kinematical arena because, when translated in terms of gravitational connections and their conjugate momenta,

[7] These are: $U(\lambda)V(\mu) = e^{i(\lambda\mu/\hbar)}\, V(\mu)U(\lambda)$ and can be obtained by setting $U(\lambda) = e^{i\lambda\hat{x}}$ and $V(\mu) = e^{i\mu\hat{p}}$ in the standard Schrödinger theory. Given a representation, $U(\lambda)$ is said to be *weakly continuous* in λ if its matrix elements between any two fixed quantum states are continuous in λ.

it requires that there be an operator corresponding to the connection itself. As we just saw, such as operator does not exist on the kinematical Hilbert space $\mathscr{H}_{\rm kin}$ of LQC; only its exponentiated versions, the holonomies, are well defined on $\mathscr{H}_{\rm kin}$. Therefore one has to develop quantum dynamics ab-initio on the new arena (see Appendix B.1).

Now in the Hamiltonian constraint of LQG, the gravitational spin connection A_a^i appears through its curvature $F_{ab}{}^i$. Since only holonomy operators are well-defined, we are led to express curvature in terms of holonomies. In the classical theory, various components of $F_{ab}{}^i$ can be obtained by first computing holonomies around appropriate (and naturally available) loops, dividing them by the areas enclosed by these loops, and taking the limit as the area shrinks to zero. In the quantum theory, the limit does not exist, reflecting that there is no local operator representing A_a^i. This, as we saw, is a distinguishing feature of LQG which lies at the heart of the discreteness of geometric operators. In particular, there is a minimum non-zero area eigenvalue—$\Delta := 4\sqrt{3}\pi\gamma\ell_{\rm Pl}^2$ in Planck units, where γ is the Barbero–Immirzi parameter—of the area operator, often referred to as the area gap. The fact that the fundamental quantum geometry has a built-in discreteness is a strong hint that we should shrink the loop only till the *physical* area it encloses is $\Delta\ell_{\rm Pl}^2$.[8]

As a consequence, the quantum curvature operator $\hat{F}_{ab}{}^i$—and hence the quantum dynamics—is now *non-local*. Locality is recovered only in the classical limit.

These considerations lead to a well-defined Hamiltonian constraint operator on the kinematical Hilbert space of LQC. It has the same form $\partial_\phi^2\Psi(v,\phi) = -\Theta\Psi(v,\phi)$ as in the WDW theory but differential operator $\underline{\Theta}_o = -12\pi G(v\partial_v)^2$ that features in the WDW constraints Eqs. (3.1) and (3.2) is now replaced by a second order *difference* operator Θ_o in v:

$$\begin{aligned}\Theta_o\Psi(v,\phi) = -F(v)\,\big(&C^+(v)\,\Psi(v+4,\phi) + C^o(v)\,\Psi(v,\phi) \\ &+ C^-(v)\,\Psi(v-4,\phi)\big)\,. \end{aligned} \tag{5.1}$$

Here, $F(v)$ and $C^\pm(v)$ and $C^o(v)$ are functions of v:

$$F(v) = \frac{3\sqrt{3\sqrt{3}}}{2\sqrt{2}}\;|v| \equiv K|v|. \tag{5.2}$$

and

$$\begin{aligned} C^+(v) &= \frac{3\pi K G}{8}\,|v+2|\;\big||v+1| - |v+3|\big|, \\ C^-(v) &= C^+(v-4) \quad \text{and} \quad C^o(v) = -C^+(v) - C^-(v). \end{aligned}$$

[8] In the μ_o framework, this area was computed using the fiducial, rather than the physical, metric (i.e., q^o_{ab} rather than q_{ab}). As we noted above the resulting quantum dynamics has a good ultra-violet behavior but a bad infra-red behavior. This is cured in the $\bar{\mu}$ scheme simply by using the physical metric to compute these areas. Secondly, in the $\bar{\mu}$ scheme, $\Delta\ell_{\rm Pl}^2$ was at first taken to be the lowest non-zero eigenvalue of the area operator, $2\sqrt{3}\pi\gamma\ell_{\rm Pl}^2$ [21; 24; 37; 56] (where γ is the Barbero–Immirzi parameter). However, it was later realized [41] that eigenstates with these eigenvalues will not appear in quantum geometries needed to represent homogeneous classical metrics. On states that can feature in this representation, the minimum non-zero eigenvalue is twice as large. Since the critical density $\rho_{\rm crit}$ at which the quantum bounce occurs in these models goes inversely as Δ, in the earlier literature, $\rho_{\rm crit}$ was $\sim 0.82\rho_{\rm Pl}$ rather than $\sim 0.41\rho_{\rm Pl}$. Both the points are discussed further in Appendix B.1.

As one might expect, the step size in the difference operator Θ_o is dictated by the area gap $\Delta \ell_{\rm Pl}^2$. There is a precise sense in which the WDW equations emerge as limits of LQC equations when Δ is taken to zero, i.e., when the Planck scale discreteness of quantum geometry determined by LQG is neglected (see Appendix B.4). Consequently, discreteness in LQC dynamics is completely negligible at late times. However, as we will see, it plays a crucial role in the Planck scale regime near singularities.

Dynamics dictated by this difference equation has been analyzed using three different methods:

- Numerical solutions of the exact quantum equations [21; 24; 30; 37]. A great deal of effort was spent in ensuring that the results are free of artifacts of simulations, do not depend on the details of how semi-classical states are constructed and hold for a wide range of parameters.
- Effective equations [24; 30; 51; 52; 53; 54]. These are differential equations which include the leading quantum corrections. The asymptotic series from which these contributions were picked was constructed rigorously but is based on assumptions whose validity has not been established. Nonetheless the effective equations approximate the exact numerical evolution of semi-classical states extremely well.
- Exact analytical results in the $k=0$, $\Lambda=0$ model [55; 56]. This analysis has provided an analytical understanding of some of the numerical results as well as several new results which are not restricted to states that are semi-classical at late times [56]. In this sense the overall picture is robust within these models.

I will now provide a global picture that has emerged from these investigations, first for the $k=1$ model without the cosmological constant Λ and for the $k=0$ case for various values of Λ. Recall that in classical general relativity, the $k=1$ closed universes start out with a big bang, expand to a maximum volume $V_{\rm max}$ and then recollapse to a big-crunch singularity. Consider a classical solution in which $V_{\rm max}$ is astronomically large—i.e., on which the constant of motion $p_{(\phi)}$ takes a large value $p_{(\phi)}^\star$—and consider a time ϕ_o at which the volume $v^\star$ of the universe is also large. Then there are well-defined procedures to construct states $\Psi(v,\phi)$ in the *physical Hilbert space* which are sharply peaked at these values of observables $\hat{p}_{(\phi)}$ and $\hat{V}|_{\phi_o}$ at the 'time' ϕ_o. Thus, at 'time' ϕ_o, the quantum universe is well approximated by the classical one. What happens to such quantum states under evolution? As emphasized earlier, there are infra-red and ultra-violet challenges:

(i) Does the state remain peaked on the classical trajectory in the low curvature regime? Or, do quantum geometry effects accumulate over the cosmological time scales, causing noticeable deviations from classical general relativity? In particular, as Green and Unruh [20] asked, is there a recollapse and if so does the value $V_{\rm max}$ of maximum volume agree with that predicted by general relativity?

(ii) What is the behavior of the quantum state in the Planck regime? Is the big-bang singularity resolved? What about the big-crunch? If they are both resolved, what is on the 'other side'?

Numerical simulations show that the wave functions do remain sharply peaked on classical trajectories in the low curvature region also in LQC. But there is a

Fig. 3 In the LQC evolution of models under consideration, the big bang and big crunch singularities are replaced by quantum bounces. Expectation values and dispersion of $|\hat{v}|_\phi$, are compared with the classical trajectory. The classical trajectory deviates significantly from the quantum evolution at the Planck scale and evolves into singularities. By contrast, the effective trajectory provides an excellent approximation to the quantum evolution at all scales. **a** The $k = 0$ case. In the backward evolution, the quantum evolution follows our post big-bang branch at low densities and curvatures but undergoes a quantum bounce at matter density $\rho \sim 0.41\rho_{\rm PL}$ and joins on to the classical trajectory that was contracting to the future. **b** The $k = 1$ case. The quantum bounce occurs again at $\rho \sim 0.41\rho_{\rm Pl}$. Since the big bang and the big crunch singularities are resolved the evolution undergoes cycles. In this simulation $p^\star_{(\phi)} = 5 \times 10^3$, $\Delta p_{(\phi)}/p^\star_{(\phi)} = 0.018$, and $v^\star = 5 \times 10^4$

radical departure from the WDW results in the strong curvature region: While the WDW evolution follows classical dynamics all the way into the big-bang and big crunch singularities (see Fig. 2), in LQC *the big bang and the big crunch singularities are resolved and replaced by big-bounces* (see Fig. 3). In these calculations, the required notion of semi-classicality turns out to be surprisingly weak: these results hold even for universes with $a_{\rm max} \approx 23\ell_{\rm Pl}$ and the 'sharply peaked' property improves greatly as $a_{\rm max}$ grows. More precisely, numerical solutions have shown that the situation is as follows (for details, see [30]).

- The trajectory defined by the expectation values of the physical observable $\hat{V}|_\phi$ in the full quantum theory is in good agreement with the trajectory defined by the classical Friedmann dynamics until the energy density ρ in the matter field is about one percent of the Planck density. In the classical solution, scalar curvature and the matter energy density keep increasing on further evolution, eventually leading to a big bang (respectively, big crunch) singularity in the backward (respectively, forward) evolution, where $v \longrightarrow 0$. The situation is very different with quantum evolution. As the density increases beyond $0.01\rho_{\rm Pl}$, quantum geometry effects become dominant, creating an effective repulsive force which rises very quickly. It then overwhelms classical gravitational attraction, and causes a bounce when ρ reaches a critical value $\rho_{\rm crit} \sim 0.41\rho_{\rm Pl}$, thereby resolving the past (or the big bang) and future (or the big crunch) singularities. Thus, there is a cyclic scenario depicted in Fig. 3.
- The volume of the universe takes its minimum value $V_{\rm min}$ at the bounce point. $V_{\rm min}$ scales linearly with $p_{(\phi)}$:

$$V_{\rm min} \propto p_{(\phi)}. \tag{5.3}$$

  Consequently, $V_{\rm min}$ can be *much* larger than the Planck size. Consider for example a quantum state describing a universe which attains a maximum radius of a megaparsec. Then the quantum bounce occurs when the volume reaches the value $V_{\rm min} \approx 5.7 \times 10^{16}\,{\rm cm}^3$, *some* 10^{115} *times the Planck volume.* Deviations from the classical behavior are triggered when the density or curvature reaches the Planck scale. The volume can be very large; it is not the variable that sets the relevant scale for quantum gravity effects.
- After the quantum bounce the energy density of the universe decreases and the repulsive force dies quickly when matter density reduces to about two percept of the Planck density. The quantum evolution is then well-approximated by the classical trajectory. On subsequent evolution, the universe recollapses both

in classical and quantum theory at the value $V = V_{\max}$ when energy density reaches a minimum value $\rho_{\min}$. $V_{\max}$ scales as the 3/2-power of $p_{(\phi)}$:

$$V_{\max} \propto p_{(\phi)}^{3/2}. \tag{5.4}$$

Quantum corrections to the classical Friedmann formula $\rho_{\min} = 3/8\pi G a_{\max}^2$ are of the order $O(\ell_{\rm Pl}/a_{\max})^4$. For a universe with $a_{\max} = 23\ell_{\rm Pl}$, the correction is only one part in 10^5. For universes which grow to macroscopic sizes, classical general relativity is essentially exact near the recollapse.

- Using ideas from geometrical quantum mechanics [57], one can obtain certain effective classical equations which incorporate the leading quantum corrections [30; 51; 52; 53]. As one would expect, quantum geometry effects primarily modify the left hand side of Einstein's equations. However, in the simplest models considered here, it is possible to rewrite the quantum corrected equation by moving the correction to the right side and then expressing it in terms of matter. This rewriting is convenient in comparing the effective equations with the classical ones. The classical Friedmann equation, $(\dot a/a)^2 = (8\pi G/3)\,(\rho - 3/8\pi G a^2)$, is replaced by

$$\left(\frac{\dot a}{a}\right)^2 = \frac{8\pi G}{3}\,(\rho - \rho_1(v))\,\left[f(v) - \frac{\rho}{\rho_{\rm crit}}\right], \tag{5.5}$$

where ρ_1 and f are specific functions of v with $\rho_1 \sim 3/8\pi G a^2$ for large a. Bounces occur when $\dot a$ vanishes, i.e., at the value of v at which the matter density equals $\rho_1(v)$ or $\rho_{\rm crit}\, f(v)$. The first root $\rho(v) = \rho_1(v)$ corresponds to the classical recollapse while the second root, $\rho = \rho_{\rm crit}\, f(v)$, to the quantum bounce. Away from the Planck regime, $f \approx 1$ and $\rho/\rho_{\rm crit} \approx 0$.

- For quantum states under discussion, the density $\rho_{\max}$ is well approximated by $\rho_{\rm crit} \approx 0.41\rho_{\rm Pl}$ up to terms $O(\ell_{\rm Pl}^2/a_{\min}^2)$, independently of the details of the state and values of $p_{(\phi)}$. (For a universe with maximum radius of a megaparsec, $\ell_{\rm Pl}^2/a_{\min}^2 \approx 10^{-76}$.) The density $\rho_{\min}$ at the recollapse point also agrees with the value $(3/8\pi G a_{\max}^2)$ predicted by the classical evolution to terms of the order $O(\ell_{\rm Pl}^4/a_{\max}^4)$. Furthermore the scale factor $a_{\max}$ at which recollapse occurs in the quantum theory agrees to a very good precision with the one predicted by the classical dynamics.
- The trajectory obtained from effective Friedmann dynamics is in excellent agreement with quantum dynamics *throughout the evolution.* In particular, the maximum and the minimum energy densities predicted by the effective description agree with the corresponding expectation values of the density operator $\hat\rho \equiv \widehat{p_{(\phi)}^2/2|p|}^3$ computed numerically.
- The state remains sharply peaked for a *very large number of 'cycles'*. Consider the example of a semi-classical state with an almost equal relative dispersion in $p_{(\phi)}$ and $|v|_\phi$ and peaked at a large classical universe of the size of a megaparsec. When evolved, it remains sharply peaked with relative dispersion in $|v|_\phi$ of the order of 10^{-6} *even after* 10^{50} *cycles of contraction and expansion!* Any given quantum state eventually ceases to be sharply peaked in $|v|_\phi$ (although it continues to be sharply peaked in the constant of motion

$p_{(\phi)}$). Nonetheless, the quantum evolution continues to be deterministic and well-defined for an infinite number of cycles. This is in sharp contrast with the classical theory where the equations break down at singularities and there is no deterministic evolution from one cycle to the next.

This concludes the summary of our discussion of the $k=1$ model. An analogous detailed analysis has been carried out also in the $k=0$ model, again with a free massless scalar field [21; 24; 37; 56]. In this case, if the cosmological constant Λ vanishes, as Fig. 1 shows, classical solutions are of two types, those which start out at the big-bang and expand out to infinity and those which start out with large volume and contract to the big crunch singularity. Again, in this case while the WDW solution follows classical trajectories into singularities, the LQC solutions exhibit a big bounce. The LQC dynamics is again faithfully reproduced by an effective equation. Again, quantum geometry modifies the left hand side of Einstein's equations but one can move this correction to the right side through an algebraic manipulation. Then, one finds that the Friedmann equation $(\dot{a}/a)^2 = (8\pi G\rho/3)$ is replaced by

$$\left(\frac{\dot{a}}{a}\right)^2 = (8\pi G\rho/3)\left(1 - \frac{\rho}{\rho_{\rm crit}}\right). \tag{5.6}$$

In classical general relativity, the right side, $8\pi G\rho/3$, is positive, whence $\dot{a}$ cannot vanish; the universe either expands forever from the big bang or contracts into the big crunch. In the LQC effective equation on the other hand, $\dot{a}$ vanishes when $\rho = \rho_{\rm crit}$ at which a quantum bounce occurs: To the past of this event, the universe is contracts while to the future, it expands. This is possible because the LQC correction $\rho/\rho_{\rm crit}$ *naturally* comes with a negative sign. This is non-trivial. In the standard brane world scenario, for example, Friedmann equation is also receives a $\rho/\rho_{\rm crit}$ correction but it comes with a positive sign (unless one artificially makes the brane tension negative) whence the singularity is not resolved.

Even at the onset of the standard inflationary era, the quantum correction $\rho/\rho_{\rm crit}$ is of the order 10^{-11} and hence completely negligible. Thus, we are justified in using classical general relativity during inflation. The quantum bounce occurs at $\rho = \rho_{\rm crit}$ and the critical density is again given by $\rho_{\rm crit} \approx 0.41\rho_{\rm Pl}$. Furthermore, one can show [56] analytically that the spectrum of the density operator *on the physical Hilbert space* admits a finite upper bound $\rho_{\rm sup}$,

$$\rho_{\rm sup} = \frac{\sqrt{3}}{32\pi^2\gamma^3 G^2\hbar}. \tag{5.7}$$

By plugging values of constants in the analytical expression of this bound, one finds $\rho_{\rm sup} = \rho_{\rm crit}$![9]

Inclusion of a cosmological constant is discussed in [39; 40]. If $\Lambda > 0$, there are again two types of classical trajectories but the one which starts out at the big-bang expands to an infinite volume at a *finite* value $\phi_{\rm max}$ of ϕ. The energy density

[9] In this evaluation, one uses the value $\gamma \approx 0.2375$ of the Barbero–Immirzi parameter γ obtained from black hole entropy calculations. The numerical simulations used to calculate $\rho_{\rm crit}$ use the same value. Because of the factor γ^{-3}, the value of $\rho_{\rm sup}$, is quite sensitive to that of γ. The fact that $\rho_{\rm sup}$ is of the order of $\rho_{\rm Pl}$ brings out a pleasing coherence between LQC and the entropy calculation from LQG.

ρ_ϕ in the scalar field goes to zero at $\phi_{\max}$. (The other trajectory is a 'time reverse' of this.) Because the ϕ 'evolution' is unitary in LQC, it yields a natural extension of the classical solution beyond $\phi_{\max}$. States which are semi-classical in the low ρ_ϕ regime again follow an effective trajectory. Since ρ_ϕ remains bounded, it is convenient to draw these trajectories in the ρ_ϕ–ϕ plane (rather than v–ϕ plane). They agree with the classical trajectories in the low ρ_ϕ regime and analytically continue the classical trajectories beyond $\rho_\phi = 0$. If $\Lambda < 0$, the classical universe undergoes a recollapse. This is faithfully reproduced by the LQC evolution. Since both the big-bang and the big-crunch singularities are resolved, the LQC evolution leads to a cyclic universe as in the $k = 1$ model. Thus, in all these cases, the principal features of the LQC evolution are robust, including the value of ρ_{crit}.

6 Discussion

Let us summarize the overall situation. In simple cosmological models, all the questions raised in Sect. 2 have been answered in LQC in remarkable detail. The scalar field plays the role of an internal or emergent time and enables us to interpret the Hamiltonian constraint as an evolution equation. The matter momentum $\hat{p}_{(\phi)}$ and 'instantaneous' volumes $\hat{V}|_\phi$ form a complete set of Dirac observables. They enable us to ask physically interesting questions. In particular, the density ρ (and the 4-d Ricci scalar) always remains bounded. In this precise sense, the big bang and the big crunch singularities are naturally resolved. On the 'other side' of the bounce there is again a large universe. General relativity is an excellent approximation to quantum dynamics once the matter density falls below a percent of the Planck density. Thus, LQC successfully meets both the 'ultra-violet' and 'infra-red' challenges. Furthermore results obtained in a number of models using distinct methods re-enforce one another. One is therefore led to take at least the qualitative findings seriously: *Big bang is not the Beginning nor the big crunch the End.* Quantum space–time appears to be vastly larger than what general relativity had us believe!

In LQC, main departures from the WDW theory occur due to *quantum geometry effects* of LQG. There is no fine tuning of initial conditions, nor a boundary condition at the singularity, postulated from outside. Also, there is no violation of energy conditions. In fact quantum corrections to the matter Hamiltonian do not play any role in the resolution of singularities of these models. John Wheeler's vision, summarized in the quote that I began this article with is realized to a surprising extent: Indeed,

> *In a finite proper time the calculated curvature rises to infinity* [in the classical theory]. *At this point the classical theory becomes incapable of further prediction. In actuality, classical predictions go wrong before this point .... The semiclassical treatment of propagation is appropriate in most of the domain of superspace of interest to gravitational collapse. Not so in the decisive region.*

Wheeler was very fond of the fundamental discreteness underlying LQG. So, he would have been pleased that it is precisely this feature that is responsible for the singularity resolution.

If no energy conditions are violated, how does this singularity resolution square with the general singularity theorems of Penrose and Hawking? They are evaded because *the left hand side* of the classical Einstein's equations is modified by the quantum geometry corrections of LQC. What about the more recent singularity theorems that Borde, Guth and Vilenkin [58] proved in the context of inflation? They do not refer to Einstein's equations. But, motivated by the eternal inflationary scenario, they assume that the expansion is positive along any past geodesic. Because of the pre-big-bang contracting phase, this assumption is violated in the LQC effective theory.

While the detailed results presented in Sect. 5 are valid only for these simplest models, partial results have been obtained also in more complicated models indicating that the singularity resolution may be robust [44] (in the sense of geodesic completeness [59]). In this respect there is a curious similarity with the very discovery of singularities in general relativity. They were first encountered in special examples. Although the examples were the physically most interesting ones—e.g., the big-bang and the Schwarzschild curvature singularities—at first it was thought that these space–times are singular because they are highly symmetric. It was widely believed that generic solutions of Einstein'e equations should be non-singular. As is well-known, this belief was shattered by the singularity theorems. Some 40 years later we have come to see that the big bang and the big crunch singularities are in fact resolved by quantum geometry effects. Is this an artifact of high symmetry? Or, are there robust *singularity resolution theorems* lurking just around the corner [59]?

A qualitative picture that emerges is that the non-perturbative quantum geometry corrections are *'repulsive'*. [10] While they are negligible under normal conditions, they dominate when curvature approaches the Planck scale and can halt the collapse that would classically have led to a singularity. In this respect, there is a curious similarity with the situation in the stellar collapse where a new repulsive force comes into play when the core approaches a critical density, halting further collapse and leading to stable white dwarfs and neutron stars. This force, with its origin in the Fermi–Dirac statistics, is *associated with the quantum nature of matter*. However, if the total mass of the star is larger than, say, 5 solar masses, classical gravity overwhelms this force. The suggestion from LQC is that a new repulsive force *associated with the quantum nature of geometry* comes into play and is strong enough to counter the classical, gravitational attraction, irrespective of how large the mass is. It is this force that prevents the formation of singularities. Since it is negligible until one enters the Planck regime, predictions of classical relativity on the formation of trapped surfaces, dynamical and isolated horizons would still hold. But one cannot conclude that there must be a singularity because the assumptions of the standard singularity theorems would be violated. There may be no singularities, no abrupt end to space–time where physics stops. Non-perturbative, background independent quantum physics would continue.

At first one might think that, since quantum gravity effects concern only a tiny region, whatever quantum effects there may be, their influence on the global

[10] We saw in Sect. 4 that there is no connection operator in LQG. As a result the curvature operator has to be expressed in terms of holonomies and becomes non-local. The repulsive force can be traced back to this non-locality. Heuristically, the polymer excitations of geometry do not like to be packed too densely; if brought too close, they repel.

properties of space–time should be negligible whence they would have almost no bearing on the issue of the Beginning and the End. However, as we saw, once the singularity is resolved, vast new regions can appear on the 'other side' ushering in new possibilities that were totally unforeseen in the realm of classical general relativity. This year we celebrate the 100th anniversary of Minkowski's celebrated paper that fused space and time into a 4-dimensional space–time continuum. It is fitting that concrete hints on what may eventually replace that continuum have begun to appear on the horizon.

Acknowledgments Much of this chapter (and all figures it contains) is based on joint work with Alex Corichi, Tomasz Pawlowski, Param Singh, Victor Taveras, and Kevin Vandersloot. I have also benefited from comments, suggestions and probing questions of many colleagues, especially Martin Bojowald, James Hartle, Jerzy Lewandowski, Donald Marolf, Roger Penrose, Carlo Rovelli and Madhavan Varadarajan This work was supported in part by the NSF grant PHY0456913, the Alexander von Humboldt Foundation, the The George A. and Margaret M. Downsbrough Endowment and the Eberly research funds of Penn State.

Appendix A: General conceptual issues

This appendix is divided into three parts. In the first I address the question of why LQC is physically interesting in spite of its drastic symmetry reduction; in the second I discuss the issue of extracting dynamics from the 'frozen formalism' and in the third I analyze Bousso's covariant entropy bound from the LQC perspective.

A.1. Why is the field of quantum cosmology interesting?

The symmetry reduction used to descend to quantum cosmology is drastic because it ignores all but finitely many degrees of freedom of the gravitational matter fields. Furthermore, it is this simplification that enables one to obtain detailed predictions in the deep Planck regime. So, a natural question arises: Why can we trust quantum cosmology? Why is it useful? More precisely, in our case, will predictions of full LQG resemble anything like what LQC predicts? This is an important question. I would like to give three arguments which suggest that the answer may be in the affirmative.

First, consider the analogy of electrodynamics. Suppose, hypothetically, that we had full QED but somehow did not have a good description of the hydrogen atom. (Indeed, it is very 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 have been that the simplification involved is so drastic that there is no reason to expect this theory to captures 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 what happened in classical general relativity. Singularities were first discovered in highly symmetric models. The general wisdom derived from the detailed analysis of the Russian 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. As noted in Sect. 6, 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. The work of the Madrid group [44] and more recent analysis of effective equations by Singh [59] suggests that the situation may be similar with singularity resolution of LQC.

Finally, the Belinskii–Khalatnikov–Lifshitz (BKL) conjecture in classical general relativity says that as one approaches space-like singularities in general relativity, 'spatial derivatives of basic fields become sub-dominant relative to the time derivatives' and dynamics at any spatial point is well approximated by that of homogeneous models, Bianchi I dynamics playing a dominant role (see, e.g., [60]). By now there is considerable support for this conjecture both from rigorous mathematical and numerical investigations.[11]

This provides some support for the idea that lessons on the quantum nature of the big-bang (and big-crunch) singularities—particularly in the Bianchi I model [41]—may be valid much more generally.

Of course none of these arguments shows conclusively that the qualitative features of LQC will remain in tact in the full theory. But they do suggest that one should not a priori dismiss LQC as being too simple.

A.2. How do you extract physics from the frozen formalism of Bergmann and Dirac?

In the 1960s and 1970s Bergmann and Komar [17; 18] pointed out that if one follows the canonical quantization procedure developed by Bergmann and Dirac, one is led to a 'frozen formalism': since physical states are solutions to the quantum constraints, (Dirac) observables must commute with the constraints and therefore appear to be constants of motion. To directly extract the dynamical content of the theory from this frozen formalism, one can adopt the following program discussed in Sects. 4 and 5:

(i) Isolate, among all dynamical variables one that can represent 'relational time' with respect to which other physical variables 'evolve'.
(ii) Introduce an appropriate scalar product on the space of solutions to the quantum constraints. This would be the physical Hilbert space $\mathscr{H}_{\rm phy}$.
(iii) Introduce on $\mathscr{H}_{\rm phy}$, a complete set of self-adjoint operators which have direct physical interpretation. These would be the Dirac observables which evolve with respect to the relational time variable.
(iv) Construct states which are semi-classical at late times, i.e., sharply peaked at a point on a classical trajectory where the matter density and curvatures are all too small for quantum gravity effects to be significant. Evolve them. Do they remain peaked on the classical trajectory in the weak curvature regime? What happens to the Dirac observables in the deep Planck regime? Do they

[11] More recently, the conjecture has been formulated in the framework one uses in LQG [61].

remain bounded or can they diverge? What is the physical interpretation of the part of the state to the 'past of the big-bang singularity'?

In LQC this program was completed as follows. As we saw in Sect. 5, in the simplest models the quantum Hamiltonian constraint takes the form

$$\partial_\phi^2 \Psi(v,\phi) = -\Theta\,\Psi(v,\phi), \tag{A1}$$

where Θ is a positive, self-adjoint *difference* operator, independent of ϕ. As explained in the main text, the form of this constraint suggests that we use ϕ as the internal or relational time variable and $\hat{V}$ (or, alternatively, matter density $\hat{\rho}$) as the physical variable which evolves with respect to ϕ. The scalar product on the space of solutions to (A1) can be introduced using the group averaging technique. Since (A1) has the same form as the Klein–Gordon equation on a static space–time, the resulting scalar product is completely analogous to that for the Klein–Gordon field. Thus, we can regard the physical Hilbert space $\mathscr{H}_{\rm phy}$ as consisting of 'positive frequency solutions' to (A1), i.e., solutions to its positive square root

$$-\,i\partial_\phi \Psi(v,\phi) = \sqrt{\Theta}\,\Psi(v,\phi). \tag{A2}$$

This has the form of the Schrödinger equation with Hamiltonian $\hat{H} = \sqrt{\Theta}$. Therefore, the inner product on the gravitational kinematic Hilbert space $\mathscr{H}_{\rm kin}^{\rm grav}$ with respect to which Θ is a positive, self adjoint operator is conserved in internal time ϕ and provides us with the physical Hilbert space $\mathscr{H}_{\rm phy}$.

Finally we can define Dirac observables. First, since $\hat{p}_{(\phi)}$ is a constant of motion, it maps physical states to physical states; it is a natural Dirac observable. The second Dirac observable is the volume operator $\hat{V}|_{\phi_o}$ at any fixed 'instant' $\phi = \phi_o$:

$$[\hat{V}|_{\phi_o}\Psi](v,\phi) = e^{i\sqrt{\Theta}(\phi-\phi_o)}\,\hat{V}\,\Psi(v,\phi_o). \tag{A3}$$

A more interesting physical observable is the density operator $\hat{\rho}|_{\phi_o}$ at the instant of time ϕ_o, defined by $\hat{\rho}|_{\phi_o} := (1/2)\widehat{V^{-1}}|_{\phi_o}\,\hat{p}_{(\phi)}^2\,\widehat{V^{-1}}|_{\phi_o}$. In the classical theory, this observable diverges as one approaches the singularity. In striking contrast, it remains bounded on the physical Hilbert space $\mathscr{H}_{\rm phy}$ [56]. Finally, as we saw in the main text, if we start with a semi-classical state in the distant future and evolve back toward the singularity using (A2), we obtain a state which is semi-classical also on the 'other side of the big-bang'. Thus, in simple cosmological models, there is a natural avenue to extract physics from the 'frozen formalism'.

A.3. Can LQC 'save' the covariant entropy bound?

Motivated by the black hole entropy formula, several entropy bounds have been proposed in the literature. The heuristic idea is the following. The leading contribution to the black hole entropy is given by (1/4)th of the area of its (isolated) horizon in Planck units. Since black holes are the 'densest' objects, one is then led to idea that if we had a complete quantum gravity theory, the number of states in any volume V enclosed by a surface of area A should be bounded by the number of states of a black hole with a horizon of area A, i.e., by $\exp A/4\ell_{\rm Pl}^2$. However, this

Fig. 4 L(B) is the portion of the future null cone of a point p up to a cross-section B such that the expansion of future directed null rays is non-negative between p and B. L(B) is a special case of a 'light sheet' that features in a more general statement of Bousso's covariant entropy bound

simple formula quickly runs into difficulties. Several improvements have been proposed. The most developed of these proposals is Bousso's covariant entropy bound [62].

The simplest version of this conjecture can be stated as follows. Let (M, g_{ab}) be a smooth classical space–time and let p be a point in it. Consider the future null cone of p and let B be any 2-sphere cross section of the null cone such that the expansion of null rays between p and B is always non-negative. Denote this portion of the null cone by L(B) (see Fig. 4). Then the Bousso's conjecture states that the entropy flux across L(B) is bounded by $A_{\rm B}/4\ell_{\rm Pl}^2$ where $A_{\rm B}$ is the area of B: $\int_{\rm L(B)} S^a dA_a \le A_{\rm B}/4\ell_{\rm Pl}^2$, where S^a is the entropy-flux 4-vector field. This statement has three curious features. First, it requires a smooth classical space–time (M, g_{ab}), without which one cannot even define null rays and their expansion. Second, it requires that the notion of the entropy-flux S^a be well defined. Finally, although it makes a crucial use of a classical metric g_{ab}, since its statement features Planck length, the conjecture is a statement about quantum gravity rather than classical general relativity. Indeed, in the limit $\hbar \to 0$ the bound becomes infinite and the conjecture trivializes. In spite of these peculiarities, however, the conjecture holds in a large number of circumstances [63; 64]. Consequently, in some particle physics circles it is taken to have deep and fundamental significance. Indeed it is sometimes stated that the covariant entropy bound is to quantum gravity what the equivalence principle was to general relativity; it should be an essential building black of any satisfactory quantum gravity theory.

Let us examine the bound in the simplest cosmological setting in classical general relativity: the $k = 0$, $\Lambda = 0$ FRW model, filled with radiation. Suppose the point p is taken to lie on a homogeneous slice $\tau = \tau_i$ and the surface B to lie on the slice $\tau = \tau_f$. Then, a straightforward calculation enables one [65] to establish the following relation

$$\frac{S}{A_{\rm B}} = \frac{\ell_{\rm Pl}^2}{6}\left(\frac{2}{45\pi}\right)^{1/4} \frac{\sqrt{\ell_{\rm Pl}}}{\sqrt{\tau_f}} \left(1 - \sqrt{\frac{\tau_i}{\tau_f}}\right). \tag{A4}$$

By plugging-in numbers, one finds that the bound $S/A_{\rm B} \le 0.25/\ell_{\rm Pl}^2$ holds if $\tau_f > 0.1\ell_{\rm Pl}$. Since $\tau_i < \tau_f$, the bound is in fact respected unless we choose the initial point p to lie *extremely* close the big-bang singularity and terminate the light cone *very* close to p. However, the bound *is* violated in the immediate future of the singularity. Usually it is argued that in this region quantum gravity effects should dominate and hence the failure of the bound cannot be taken seriously; quantum corrections will intervene and save the bound.

Is this really the case? A priori this possibility seems almost impossible to test because of the three peculiar features I mentioned above. On the one hand, quantum gravity effects are essential. On the other, if they lead to significant fluctuations in the space–time metric, one loses even the formulation of the conjecture! Surprisingly, LQC provides an ideal arena to test this possibility because of the following two features. First, quantum corrections can indeed intervene; they are so strong that the singularity is resolved. Second, in spite of these strong effects, there is a smooth metric even at the bounce at which the quantum state is sharply peaked. This is not the metric given by Einstein's equations but rather by the LQC effective equations which incorporate the quantum corrections that unleash the tremendous repulsive force of quantum geometric origin. Still, since there is a smooth metric, the conjecture is meaningful and can therefore be tested. A detailed calculation [65] shows:

$$\frac{S}{A_{\mathrm{B}}} < \frac{0.244}{\ell_{\mathrm{Pl}}^2}. \tag{A5}$$

Thus in LQC the bound is in fact respected. Although the calculation has several limitations (see [65]), it nonetheless provides an interesting and completely unforeseen convergence of very different ideas related to quantum gravity.

This result suggests the following overall viewpoint on the entropy bound. Recall that the bound is strongly motivated by the generalized second law of thermodynamics (which also does not have a sharp, definitive formulation). Now, already the standard second law of thermodynamics is a deep fact of Nature but it has a 'fuzziness' which is not shared by other deep laws such as energy-momentum conservation. In particular, the second law requires a coarse graining in an essential way. It is not a statement about the evolution of micro-states; in a fundamental theory their dynamics is always time reversible (leaving aside, for simplicity, quantum measurements). Rather, it is a statement about how the number of micro-states compatible with a pre-specified coarse graining changes in time. For specific processes, the increase of entropy can be calculated using statistical mechanics. But this entropy has little relevance to the fundamental dynamics of micro-states and is not an *input* in the construction of statistical mechanics. In the same vein, it seems unlikely that covariant entropy bounds would be essential ingredients in the *construction* of a quantum theory of gravity. It seems more natural to expect the covariant entropy bound should *emerge* from a fundamental quantum gravity theory under suitable conditions. Returning to the LQC calculation, the distinguishing feature of LQC is the underlying quantum geometry. The covariant entropy bound was never an input or even a motivation. Rather, it emerged on the quantum corrected semi-classical space–time that results from the LQC dynamics.

Appendix B: Quantum dynamics

This appendix is divided into four parts. In the first I discuss how the Hamiltonian constraint is handled in LQC. In the second, I point out that, although the difference between the 'μ_o and $\bar{\mu}$ schemes' is quite subtle, the resulting quantum constraints have very different predictions. Quantum dynamics resolves the singularity in both cases but the μ_o scheme leads to inadmissible infrared behavior. This difference has valuable lessons for the construction of the quantum Hamiltonian constraint in full LQG. In the third, I summarize the analytical results that provide a precise sense in which the singularity is resolved in the $\bar{\mu}$ scheme. In the fourth, I will conclude by providing a precise relation between the results of LQC and those of the WDW theory.

B.1. How is dynamics handled in LQC?

The Hamiltonian constraint has the following form in full LQG:

$$C_{\rm H} \sim \underbrace{(\varepsilon^{ij}{}_k E^a_i E^b_j/\sqrt{q})}_{\rm Triads} \; \underbrace{F^k_{ab}}_{\rm connection} , \qquad \text{(B1)}$$

where the first term is determined by spatial triads E^a_i and the second by the gravitational spin connection A^i_a. To define quantum dynamics, we have to first find the corresponding operator $\hat{C}_{\rm H}$ on the kinematical Hilbert space $\mathscr{H}_{\rm kin}$ of LQC. Thanks to a general procedure introduced by Thiemann, we know how to handle the first term involving triads. That procedure has a direct analog in LQC (see, e.g., [33]). However, the second term poses a challenge: Although the curvature ${F_{ab}}^k$ has a simple expression in terms of A^i_a, as we saw in Sect. 4, there is no operator corresponding to the connection either in LQG or LQC.

But the holonomy operators are well defined in both theories. Indeed they are the fundamental/elementary configuration operators on $\mathscr{H}_{\rm kin}$. Now, to quantize a function f on any phase space, the standard strategy in quantum physics is to first express f as a suitable function of the elementary configuration and momentum variables and then replace each of these variables by its quantum analogs. Modulo factor ordering, this procedure yields the desired quantum operator $\hat{f}$. It is natural to follow this procedure to obtain the operator ${\hat{F}_{ab}}{}^k$. The first step is straightforward. For, the a–b component of curvature at a point p can be expressed in terms of the holonomy $h_\Box$ around a closed loop $\Box$ in the a–b plane at p as a limit,

$$F^k_{ab} = -2 \lim_{{\rm Ar}_\Box \to 0} \frac{{\rm Tr}(h_{\Box_{ab}} - 1)\tau^k}{{\rm Ar}_\Box}, \qquad \text{(B2)}$$

in which the area of the 2-surface enclosed by the loop $\Box$ tends to zero. In the second step we can to replace the holonomy $h_\Box$ by the operator $\hat{h}_\Box$ on $\mathscr{H}_{\rm kin}$. However, as we shrink the loop, the limit of this operator does not exist on $\mathscr{H}_{\rm kin}$. This is not accidental but is tied to the fundamental feature of the unique Hilbert space $\mathscr{H}_{\rm kin}$ we are led to by the requirement of diffeomorphism covariance [34; 35]. Indeed, had this limit existed, we would have had a local operator corresponding to the gravitational connection A^i_a. Now, in full LQG, this difficulty can be bypassed by first solving the diffeomorphism constraint and then working on the space $\mathscr{H}_{\rm diff}$ of diffeomorphism states rather than $\mathscr{H}_{\rm kin}$. On these diffeomorphism invariant states Ψ, we can easily shrink the loop because, once the loop is sufficiently small, $\hat{h}_\Box \Psi$ remains invariant under the operation of shrinking the loop further.

In LQC, on the other hand, since we have eliminated the diffeomorphism constraint by gauge fixing, we have to work directly on $\mathscr{H}_{\rm kin}$. Therefore, to define $\hat{F}^k_{ab}$, one adopts the following working strategy [33]. Recall that in LQG the connection operator is not well-defined because the holonomy fails to be weakly continuous in the loop and it is precisely this lack of continuity that leads one to quantum geometry in which geometric operators—particularly areas of surfaces—have purely discrete eigenvalues. This interplay is taken to suggest that we have to take the quantum nature of geometry seriously. We cannot shrink the loop to zero area continuously. Rather, we should define $\hat{F}^k_{ab}$ simply by evaluating $\hat{h}_\Box$ in the operator analog of (B2) around a loop $\Box$ which encloses an area equal to the smallest non-zero eigenvalue $\Delta\ell_{\rm Pl}^2$ of the area operator, called the *area gap*. The resulting operator is an acceptable quantization of $\hat{F}_{ab}{}^k$ because is has the correct classical limit F_{ab}^k in a precise sense. However, at a fundamental level the operator has a *Planck scale non-locality*. It is only in the classical limit that it reduces to the familiar local form $F_{ab}{}^k = 2\partial_{[a}A_{b]} + \varepsilon_{ij}{}^k A_a^i A_b^j$.

The technical implementation of this idea involves two subtleties that were overlooked in the beginning. In the first implementation [33], the loop $\Box$ was chosen so that the area it encloses with respect to the *fiducial* metric is $\Delta\,\ell_{\rm Pl}^2$. This is called *the* μ_o *scheme*. It led to a quantum constraint that resolves the singularity [21]. However, as we will see in Appendix B.2, it has severe limitations. In particular, it predicts deviations from general relativity even in certain 'tame' situations. However it was soon realized that these difficulties go away if, in the construction of $\hat{F}_{ab}{}^k$ the area enclosed by $\Box$ is computed using the *physical* metric q_{ab} rather than the fiducial metric ${}^oq_{ab}$ [24]. This switch is conceptually well motivated since quantization of area eigenvalues refers to the actual metric used in the LQG kinematics, not an auxiliary or a fiducial one. This strategy is referred to in the literature as *the* $\bar{\mu}$ *scheme*. While the technical implementation of this strategy is rather subtle, the final Hamiltonian constraint (5.1) is a rather simple difference operator in the volume variable v. As one might expect, the step size of the operator is dictated by the area gap.[12]

In the limit in which the gap goes to zero, this quantum constraint (5.1) reduces to the Hamiltonian constraints (3.1) and (3.2) of the WDW theory in the sense spelled out in Appendix B.4.

The second subtlety is less significant. In much of the literature [24; 30; 31; 38; 56] the area gap $\Delta\ell_{\rm Pl}^2$ was taken to be $2\sqrt{3}\pi\gamma\ell_{\rm Pl}^2$, the lowest of all non-zero eigenvalues of the area operator on $\mathscr{H}_{\rm kin}$ (where γ is the Barbero–Immirzi parameter). However, it was later realized [41; 65] that, if one uses a semi-heuristic correspondence between LQG and LQC states, LQG eigenstates with these eigenvalues will not appear in quantum geometries needed to represent homogeneous classical metrics. On states that can feature, the minimum non-zero eigenvalue is *twice as large*. This shift has no qualitative effect on the earlier results in the $\bar{\mu}$ scheme (e.g., those in [24; 30; 31; 38; 56]). The only difference is a factor of 2 in some expressions. In particular, the critical density $\rho_{\rm crit}$ at which the quantum bounce occurs in these models goes inversely as Δ, whence in the earlier literature, $\rho_{\rm crit}$ was $\sim 0.82\rho_{\rm Pl}$ rather than $\sim 0.41\rho_{\rm Pl}$.

Note that I have referred to this construction as a 'working strategy'. This is because one has to 'parachute' into LQC certain important facts about quantum geometry from the kinematics of full LQG. This is analogous to Bohr's treatment of the hydrogen atom where, in retrospect, one can say that quantization of angular momentum is 'parachuted' into the model from full quantum mechanics. With incorporation of this one essential feature, the simple Bohr model is capable of giving energy levels to a remarkable accuracy. However, at a fundamental level, one has to use full quantum treatment a la Pauli or Schrödinger. Similarly, in

[12] In the μ_o scheme, the 'lattice' has uniform spacing in p, the variable which measures the area of each surface of the fiducial cell while in the $\bar{\mu}$ scheme it has uniform spacing in volume v. Since $v \sim p^{3/2}$, the dynamics of $\bar{\mu}$ scheme cannot be supported by alternative LQC kinematics of the type proposed by Velhinho [66].

quantum cosmology a more fundamental construction will emerge only from a better understanding of the detailed relation between LQG and LQC.

B.2. What are the differences between the μ_o and $\bar{\mu}$ quantum theories?

Recall, first, that in the $k = 0$ model on $\mathbb{R}^3$, it is often convenient to introduce a fiducial metric q^o_{ab} and label the physical metric q_{ab} via a scale factor $a(t)$: $q_{ab} = a^2(t)\, q^o_{ab}$. If we rescale the fiducial metric via $q^o_{ab} \to \alpha^2\, q^o_{ab}$, the descriptor a of the physical metric q_{ab} changes via $a \to \alpha^{-1} a$ even though q_{ab} itself is untouched. Of course physics can not change under such rescalings. The construction of a Hamiltonian or Lagrangian framework requires an additional auxiliary structure because one has to perform integrals of physical fields over space and these diverge because of homogeneity. Therefore, one has to introduce a fiducial cell $\mathscr{C}$ and restrict all integrals to $\mathscr{C}$. In classical general relativity, one can work directly with field equations and the auxiliary $\mathscr{C}$ is unnecessary. However it is essential for passage to quantum theory, irrespective of whether one uses path integrals or canonical quantization.

Thus, in any quantum cosmology on non-compact, spatially homogeneous manifolds, there are two independent auxiliary structures, the metric q^o_{ab} and the cell $\mathscr{C}$. Each can be changed keeping the other fixed. At the classical level, the final physical results do not depend on the specific choices one makes to construct the Hamiltonian theory. But a priori there is no guarantee that results of the quantum theory will continue to enjoy this feature. If they do not in a specific quantum theory, that theory cannot be physically viable. The first contrast between the two schemes is that while in the μ_o scheme the final results of the quantum theory depend on these auxiliary structures[13], in the $\bar{\mu}$ scheme they do not.

Since a cell $\mathscr{C}$ is in any case necessary to the Hamiltonian framework, one can make kinematics manifestly independent of the fiducial metric q^o_{ab} by rescaling the canonical variables by suitable powers of the volume V_o of $\mathscr{C}$ with respect to q^o_{ab} [33]. Then the canonical commutation relations, and expressions of the elementary operators are all independent of the choice of q^o_{ab}. Thus, for each choice of $\mathscr{C}$ one constructs a quantum theory. Now, suppose we are given a classical solution $(a(t), \phi(t))$. Within each quantum theory, one can construct semi-classical states peaked at this solution at a late time when curvature is low and evolve it back in time. One can then ask: when do quantum effects become important? Unfortunately, in the μ_o scheme, the answer depends on the choice of the cell $\mathscr{C}$! (see Appendix B.2 in [24]). In particular, the matter density ρ_b at the bounce point is given by $\rho_b = (3/8\pi G\gamma^2\mu_o^2)^{3/2}\, (\sqrt{2}/p_{(\phi)}) \equiv C/p_{(\phi)}$ where by inspection the constant C does not depend on the choice of $\mathscr{C}$ (or q^o_{ab}). However, since $p_\phi = \dot{\phi}\, V$ where V is the physical volume of $\mathscr{C}$, ρ_b decreases linearly with the size of $\mathscr{C}$. Thus, in the μ_o scheme, even the density at the bounce point fails to have a physical meaning. By contrast, in the $\bar{\mu}$ scheme, ρ_b is universal, independent of the choice of $\mathscr{C}$.

[13] It is often possible to hide the dependence on the choice of q^o_{ab} by shifting it to the choice of the cell $\mathscr{C}$ or vice versa but of course physics has to be invariant with respect to both these choices.

A second difference is that the μ_o scheme has serious problems with recovering general relativity in the low curvature limit while the $\bar{\mu}$ scheme is free of this drawback. To see this, let us fix a cell $\mathscr{C}$ and examine the resulting quantum theory. As we just saw, in the $k = 0$, $\Lambda = 0$ case, the matter density at the bounce point is given by $\rho_b = C/p_{(\phi)}$. Now, p_ϕ is a constant of motion and larger its value, more semi-classical the state is. (For example, as we saw in Sect. 5, in the $k = 1$ case the maximum radius of the universe goes as $p_{(\phi)}^{3/2}$.) So, ρ_b can be made as low as we want simply by increasing $p_{(\phi)}$. In particular, there are states which are extremely semi-classical at late times which, when evolved back undergo a quantum bounce at density of water! A gross violation of general relativity at such densities is clearly unphysical. In the $\bar{\mu}$ scheme on the other hand, $\rho_b \approx 0.41\rho_{\rm Pl}$ is universal, irrespective of how large $p_{(\phi)}$ is.

A third difference between the two schemes arises in presence of a cosmological constant. If $\Lambda \neq 0$, problems with the infra-red behavior also arise in the μ_o scheme *well away from the bounce*. Even at late times, the quantum theory exhibits large departures from general relativity in low curvature regimes. Again, this cannot happen in the $\bar{\mu}$ scheme. It is quite remarkable that a subtle but physically well-motivated correction in the construction of the quantum field strength operator cures all the conceptual and physical pathologies of the μ_o scheme without affecting the singularity resolution. It is a marvelous example of the deep harmony between physics and mathematics.

The difference between the two schemes also has important lessons for full LQG. Recently, Giesel et al. [67; 68] have pioneered a program to deparametrize general relativity along the lines of Brown and Kuchař [69], making the treatment of constraints in LQG conceptually similar to that in LQC. This is a notable advance. However, quantization of the Hamiltonian constraint continues to face a host of ambiguities in full LQG. The fact that the apparently natural μ_o scheme is not viable even in the simplest LQC models suggests that a much greater control on the semi-classical predictions is needed to weed out ambiguities. Specifically, an understanding the relation between choices made in the quantization of the Hamiltonian constraint and the behavior of the resulting physical states in the semi-classical regime would go a long way to reducing the large apparent freedom one is currently faced with.

Finally, in this appendix I have spelled out differences between the μ_o and $\bar{\mu}$ schemes in general terms because the more complete discussion of [24; 38; 56] is rather technical. As a result, it appears not to have been fully absorbed by the community and some authors continue to treat the two schemes on an almost equal footing.

B.3. Are there analytical results that elucidate properties of the quantum bounce?

There are two analytical results that are particularly interesting because they zero-in on the key features of the bounce: the first provides an upper bound on the spectrum of the matter density operator in LQC and the second shows that the 'bounce' is not restricted to states which are semi-classical at late times but occurs for all states in the domain of the volume operator.

In the first papers [21; 37] on the bounce, the analysis began with the choice $N = 1$ of the lapse function. In the classical theory the corresponding Hamiltonian constraint generates evolution in proper time. One then found the quantum operator corresponding to this constraint. But as we saw, physical interpretation of the theory is simplest if one uses the scalar field ϕ as internal time. The corresponding lapse is $N = V$, the volume of the fiducial cell with respect to the physical metric q_{ab}.[14]

One can begin with this lapse already in the classical theory and then quantize. If one does so, the constraint is simpler because it does not involve any inverse powers of V (even if one were to include dust, radiation or other kinds of matter used in the cosmology literature). This strategy was not adopted in the first papers because, if the underlying 3-manifold is non-compact, the strategy does not naturally generalize to inhomogeneous contexts. However, it has some conceptual and technical advantages in homogeneous cosmologies. In fact the quantum constraint coincides with that of the so-called simplified LQC—called sLQC in the literature—*which can be solved exactly analytically* [56]. sLQC itself was first arrived at by first using $N = 1$, going to the quantum theory and then making certain simplifications in the resulting quantum constraint [56]. This round-about procedure is not necessary. One arrives at the same exactly soluble quantum theory if one formulates the classical theory with $N = V$, i.e., with the scalar field as internal time, and then proceeds with quantization.

Since this theory is exactly soluble, one can establish several interesting results analytically. First consider the matter density operator $\hat{\rho}|_\phi = \frac{1}{2}\,(\hat{V}_\phi)^{-1}|_\phi\; \hat{p}^2_{(\phi)}\; (\hat{V}_\phi)^{-1}|_\phi$ at the instant ϕ of the internal time. One can show that its spectrum has an absolute upper bound $\rho_{\rm sup}$ *on the physical Hilbert space* [56]:

$$\rho_{\rm sup} = \frac{\sqrt{3}}{16\pi^2\gamma^3 G^2\hbar} \approx 0.41\rho_{\rm Pl}. \tag{B3}$$

Since the inverse volume operator $\widehat{V^{-1}}$ is bounded above, already on the kinematic Hilbert space $\mathscr{H}_{\rm kin}$, $\hat{\rho}$ is bounded above *provided one restricts oneself to the subspace of the Hilbert space spanned by the eigenstates of $\hat{p}_{(\phi)}$ with eigenvalues below any fixed $p^o_{(\phi)}$*. This kinematical result is sometimes used to argue that singularity is resolved (see, e.g., [70]). However, since the full spectrum of $\hat{p}_{(\phi)}$ is *un*bounded above, so is $\hat{\rho}$ on $\mathscr{H}_{\rm kin}$. The fact that it admits an absolute upper bound on $\mathscr{H}_{\rm phy}$ does not follow from the boundedness of $\widehat{V^{-1}}$; it is a highly non-trivial consequence of *quantum dynamics.* It provides a clear-cut sense in which the singularity is resolved in LQC.

It is natural to ask: How good is this bound $\rho_{\rm sup}$? Is it actually achieved? Using states which are Gaussians at late times, one can show that the expectation values $\rho_{\rm bounce}$ of the density operator at the bounce point approach arbitrarily close to

[14] This corresponds to working in the harmonic-time gauge: on space–time $ds^2 = -a^3(T)V_o dT^2 + a^2(T)d\vec{x}^2$, the time coordinate T satisfies the wave equation and the scalar field $\phi(T)$ is given by $\phi(T) = (p_{(\phi)}/V_o)T$ (where V_o is the volume of the cell $\mathscr{C}$ with respect to the fiducial metric q^o_{ab} and p_ϕ is a constant of motion).

ρ_{sup}:

$$\rho_{\text{bounce}} = \rho_{\text{sup}} \left[1 - O\left(\frac{G\hbar^2}{p_{(\phi)}^2 + (\Delta p_{(\phi)})^2} \right) \right], \tag{B4}$$

where $\Delta p_{(\phi)}$ is the dispersion in $\hat{p}_{(\phi)}$ Thus, ρ_{sup} is indeed the lowest upper bound on the spectrum of the density operator. Chronologically, ρ_{bounce} was first found in numerical simulations. It turned out to be remarkably robust in the sense that it is insensitive to modeling of the semi-classical states in three different ways and does not alter when a non-zero cosmological constant is included [24; 39; 40] or when the analysis is extended to the $k = 1$ case [30]. This robustness suggested that there must be an analytical result that $\hat{\rho}$ is a bounded operator, which indeed turned out to be the case. This is a nice example of the synergistic interplay between numerical and analytical work.

Finally, we can ask if the quantum bounce is restricted only to states which are semi-classical at late times. On general states, one has to first define what one means by a bounce. A natural strategy is to examine expectation values of the volume operator. In the exactly soluble model, one finds [56] that for *any state in the domain of the volume operator* we have:

$$(\Psi, \hat{V}_\phi \Psi)_{\text{Phy}} = V_+ e^{\sqrt{12\pi G}\phi} + V_- e^{-\sqrt{12\pi G}\phi}, \tag{B5}$$

where $V_\pm$ are determined by the 'initial data' $\Psi(v, \phi_o)$ for the state at any ϕ_o. Therefore, it follows that the expectation value is well-defined for all finite times ϕ but grows unboundedly as $\phi \to \pm\infty$. Hence it must attain a minimum. Indeed, the minimum is given by:

$$V_{\text{min}} = \sqrt{(V_- V_+)} \tag{B6}$$

and occurs at time $\phi_{\text{bounce}} = \frac{1}{2\sqrt{12\pi G}} (\ln V_- - \ln V_+)$.

B.4. What is the precise relation between the LQC and the WDW dynamics?

This question has been analyzed in detail for the exactly soluble theory (i.e., the $k = 0, \Lambda = 0$ model) I just discussed in Appendix B.3. Let us start with a physical state at a late time $\phi = \phi_o$ when the matter density and curvature are low, evolve it using LQC and the WDW theory and compare the results. In the LQC evolution, the area gap $\Delta \ell_{\text{Pl}}^2$ plays a key role while in the WDW theory, it is effectively zero. To compare the two evolutions, let us not fix $\Delta \ell_{\text{Pl}}^2$ to its numerical value $4\sqrt{3}\pi\gamma\ell_{\text{Pl}}^2$ used in LQC but allow Δ to vary so we can take the limit $\Delta \to 0$. Then:

- Certain predictions of sLQC approach those of the WDW theory as Δ goes to zero. That is, given a semi-infinite 'time' interval I_ϕ and an $\varepsilon > 0$, there exists a $\delta > 0$ such that $\forall \Delta < \delta$, 'physical predictions of the two theories are within ε of each other' if restrict ϕ to lie in I_ϕ.
- However, approximation is *not* uniform. The WDW theory is *not* the limit of LQC as Δ goes to zero. Thus, given $N > 0$ however large, there exists a ϕ such that $\langle \hat{V}_\phi \rangle_{\text{sLQC}} - \langle \hat{V}_\phi \rangle_{\text{WDW}} > N$. In this sense, LQC is *fundamentally* discrete.

Thus the relation is somewhat more subtle than one might have first thought. If we are interested in physical predictions either to the past or to the future of any fixed time $\phi = \phi_o$, LQC does reduce to the WDW theory in the limit in which the area gap is taken to zero. But the WDW theory is *not* the 'continuum limit' of LQC because if we include the full time interval, there are many physical predictions of LQC which will not reduce to those of the WDW theory. In fact, as a full fledged theory, LQC does not admit a continuum limit; it is a fundamentally discrete theory. For more precise and detailed statements, see [56].

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