Numerical Analysis of the Big Bounce in Loop Quantum Cosmology

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Loop quantum cosmology homogeneous models with a massless scalar field show that the big-bang singularity can be replaced by a big quantum bounce. To gain further insight on the nature of this bounce, we study the semi-discrete loop quantum gravity Hamiltonian constraint equation. For illustration purposes, we establish a numerical analogy between the quantum bounces and reflections in finite difference discretizations of wave equations triggered by the use of nonuniform grids or, equivalently, reflections found when solving numerically wave equations with varying coefficients.

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

Motivated by understanding the differences between various ambiguities in the constraints for the full theory, we will show that the observed turning point is strongly tied to the method to carry out the temporal updating of the system. Specifically, explicit time-update of the semi-discrete Eq. 1, such as the 4th-order Runge-Kutta updating used in Refs. 7, 8, 9, will yield a bounce. One can draw a numerical analogy in which the bounce can be understood in the context of spurious reflections from finite difference discretizations of wave equations in nonuniform grids 11 or equivalently from numerical solutions to wave equations with varying coefficients. Bounces due to discreteness have been also obtained in the study of Hawking radiation on a falling lattice 12.

We first introduce the standard mesh-index notation used in finite differences, namely \( v_j = j \Delta v \) with \( \Delta v = 4 v_o \). In this notation, the semi-discrete Eq. (1) takes the form

\[
\partial^2_{\phi} \Psi_j = \frac{3}{2} \kappa B^{-1}(v) \left( C(v + 2v_o) \left[ \Psi(v + 4v_o) - \Psi(v) \right] - C(v - 2v_o) \left[ \Psi(v) - \Psi(v - 4v_o) \right] \right),
\]

where \( B(v) = 3|v| |v + v_o|^{1/3} - |v - v_o|^{1/3}^3 \) is related to the eigenvalues of the inverse volume operator \( 10 \) and \( C(v) = |v| |v + v_o| - |v - v_o|/4 \). Units are such that \( \kappa \equiv 8\pi G \). In Eq. (1), it is implied that \( \Psi \) also depends on \( \phi \). The discrete independent variable \( v \) is the eigenvalue of the volume operator, with the discretization scale \( v_o \) fixed by the area gap. The scalar field \( \phi \) is used as an internal time. Starting with a state that is semi-classical at late times, evolutions backwards in time using Eq. (1) yield a turning point, a quantum bounce, before reaching the classical singularity at \( v = 0 \) [9]. The turning point takes place when the total energy density reaches a critical value \( \rho_{\text{crit}} < \rho_{\text{Planck}} \).

The goal of this Letter is to gain further insight, from a numerical analysis point of view, about the nature of this bounce. We will show that the observed turning point is strongly tied to the method to carry out the temporal updating of the system. Specifically, explicit time-update of the semi-discrete Eq. (1), such as the 4th-order Runge-Kutta updating used in Refs. 7, 8, 9, will yield a bounce. One can draw a numerical analogy in which the bounce can be understood in the context of spurious reflections from finite difference discretizations of wave equations in nonuniform grids 11 or equivalently from numerical solutions to wave equations with varying coefficients. Bounces due to discreteness have been also obtained in the study of Hawking radiation on a falling lattice 12.

Motivated by understanding the differences between various ambiguities in the constraints for the full theory, we will also show that the bounce could be avoided by introducing an implicit time-update, which is formally equivalent to adding ad hoc higher order terms to the LQC Hamiltonian constraint. With this implicit update, it is possible to evolve backwards in time a state that reaches the classical big-bang singularity. At that point, the wavefunction \( \Psi \) gets partially reflected and partially transmitted through the singularity. The resulting evolution is deterministic and thus also resolves the problem of the big-bang singularity.

We first introduce the standard mesh-index notation used in finite differences, namely \( v_j = j \Delta v \) with \( \Delta v = 4 v_o \). In this notation, the semi-discrete Eq. (1) takes the form

\[
\partial^2_{\phi} \Psi_j = \frac{3}{2} \kappa \tilde{B}^{-1} D_{\psi} \tilde{C} D_{\psi} \Psi_j
\]

where \( \tilde{B} = (3|v|^{1/3} \tilde{D}_{\psi}|v|^{1/3}/|v|) \) and \( \tilde{C} = |v| \tilde{D}_{\psi}|v| \) with \( D_{\psi} f_j \equiv (f_{j+1/2} - f_{j-1/2})/\Delta v \) and \( \tilde{D}_{\psi} f_j \equiv (f_{j+1/4} - f_{j-1/4})/\Delta v/2 \) discrete finite difference operators. In
the limit $\Delta v \to 0$, both of these operators become $\partial_v$ as well as $\tilde{B} \to 1/[v]$ and $\tilde{C} \approx 1/[v]$. Also in that limit, Eq. $[2]$ becomes $\partial^2_v \Psi = 3k\nu/2\partial_v(\nu(v\dot{\Psi})$; that is, one recovers the WDW equation in the $v \propto a^3$ representation where $a$ is the scale factor.

To simplify our analysis, we will work with a version of Eq. $[2]$ in which $\tilde{B} \approx 1/[v]$ and $\tilde{C} \approx 1/[v]$; that is, $\partial^2_v \Psi_j = (3k/2)v\partial_v(\nu D_v(\nu(\partial_v \psi_j)))$. The differences between this equation and Eq. $[2]$ are of $O(\Delta v^2)$ and do not affect our conclusions regarding the big quantum bounce. In addition, since ultimately the mean trajectories of states in the $\phi-v$ plane are given by the characteristic of $\partial^2_\phi \Psi_j = (3k/2)v\partial_v(\nu D_v(\nu(\partial_v \psi_j)))$, we will concentrate our attention on its principal part, namely $\partial^2_\phi \Psi_j = c^2 D^2_v \Psi_j$

where $c = \sqrt{3k/2v}$.

The starting point of our analysis is applying a time-Fourier transformation $\Psi_j(\phi) = \int_{-\infty}^{\infty} e^{-i\omega \phi} \tilde{\Psi}_j(\omega) d\omega$.

Thus, $-\omega^2 \tilde{\Psi}_j = c^2 D^2_v \tilde{\Psi}_j$. Next, we insert the plane wave solutions $\tilde{\Psi}_j \pm 1 = e^{\pm ik\Delta v \tilde{\Psi}_j}$ with wavenumber $k$. For $\Delta v^2/2c \leq 1$, this yields the following dispersion relationship

$$\Delta v \omega/2c = \pm \sin \left(\frac{\Delta v k}{2}\right).$$

For $\Delta v/2c > 1$, the wave is exponentially damped. From this dispersion relation, the group velocity $V_g = d\omega/dk$ is given by

$$V_g = \pm c \cos \left(\frac{\Delta v k}{2}\right) = \pm c \left[1 - \left(\frac{\Delta v \omega}{2c}\right)^2\right]^{1/2}.$$

It is then clear that the states, solutions of the semi-discrete equation, will have different dynamics from those of the continuum WDW equation. WDW states have a group velocity $\pm c$ and follow characteristics $v = v_\nu \pm \sqrt{3/2(\phi - \phi_\nu)}$ with $v_\nu$ and $\phi_\nu$ integration constants. On the other hand, LQC states have group velocity $V_g |V_g| \leq c$ and mean trajectories $v = \xi/2e^{\pm \sqrt{3/2(\phi - \phi_\nu)}} + (v_\nu/\xi)^2 e^{\pm \sqrt{3/2(\phi - \phi_\nu)}}$, with $\xi = \nu_\nu + \sqrt{v_\nu^2 - v_b^2}$ and $v_b = \Delta v \omega/\sqrt{6k}$. The value $v_b$ is the location where the group velocity vanishes. This is where the characteristics reverse direction, the big quantum bounce. The condition $(\Delta v^2/2c)^2 = 1$ is precisely the condition $\rho/\rho_{\text{crit}} = 1$ for the quantum bounce derived in Ref. $[9]$ after identifying $\omega$ with $P_\phi$, the momentum conjugate to “time.”

Applying an identical analysis to the version of LQC Hamiltonian constraint in Ref. $[5, 8]$, one arrives to Eq. $[7]$ with $v$ replaced by the triad $p$ and setting $c = \sqrt{2\kappa/3|p|}$. The location of the bounce is now at $p_b = \Delta \nu \omega/\sqrt{6k/3}$. Since $v \propto a^{3/2} \propto a^3$, when translated to the $a$ representation, the turning points $v_b$ and $p_b$ occur at different values of $a$, or equivalently, for different total energy densities $\rho_{\text{crit}}$. This “coordinate transformation” was the key ingredient in Ref. $[9]$ for having the bounce occurring at $\rho_{\text{crit}} < \rho_{\text{Planck}}$.

It is very important to emphasize that the derivation of $V_g$ and its turning point condition did not depend on any specific time-update (e.g. Staggered Leap-Frog, Crank-Nicholson, Runge-Kutta, etc). The only two assumptions used were the “spatial” discretization in Eq. $[1]$ or $[2]$, i.e. centered second order accurate finite differences, and that the time-update is explicit; that is, the numerical approximation to $\partial^2_\phi \Psi_j$ was assumed to depend only on $j$. In other words, the l.h.s. of Eq. $[1]$ or $[2]$ only depends on $v_j$. From the LQC point of view, the explicit time-update arises because the inverse scalar factor operator used in deriving Eq. $[1]$ is diagonal. Also important is to keep in mind that, since the truncation errors from approximating $\tilde{B} \approx 1/[v]$ and $\tilde{C} \approx 1/[v]$ are small and only become relevant in the immediate vicinity of the classical singularity, the bounce observed from the LQC equation would be identical to that from solving numerically the WDW equation with second order center difference approximations and explicit time-integration. In this regard, what distinguishes LQC and WDW equations is the specific forms of the spatial operators, continuum operators for WDW and discrete for LQC.

A possible way of avoiding the bounce in the discrete WDW equation is to perform the coordinate transformation $\alpha \propto \ln a \propto \ln \nu^{1/3}$. With this transformation, the WDW equation becomes $\partial^2_\phi \Psi = c^2 \partial^2_\phi \Psi$ with $c = \sqrt{\kappa/6}$. Using a uniform mesh in $\alpha$, the group velocity in this case is identical to $[4]$ with $\Delta v$ replaced by $\Delta \alpha$. Thus, provided the initial state satisfies $\Delta \alpha \omega/2c < 1$, the group velocity will not vanish. The same coordinate transformation can be applied to the LQC Eq. $[1]$, however, because the LQC theory requires keeping $\Delta v$ constant, the mesh in the $\alpha$ coordinate will not be uniform. It is in this context that one can view the bounce as spurious reflections due to nonuniform grids $[11]$.

So far, we have only revisited the semi-discrete LQC Eq. $[11]$ under the numerical analysis eyepiece. In particular, we have demonstrated that the nature of the quantum bounce is not entirely due to the specific form of the “spatial” operator in the r.h.s. of the equation, which is the main difference between the LQC and WDW equations. Also very important, and closely intertwined for the appearance of the bounce, is the explicit time-update implied by l.h.s. of the difference equation. If time-updates play a crucial role, one could ask whether other time-updates could radically change the dynamics, and in particular the bounce, while keeping fixed the spatial discretization. The answer is affirmative.

Let us consider the following modification to Eq. $[2]$,

$$M_r^2 \partial^2_\phi \Psi_j = \frac{3}{2} \kappa \tilde{B}^{-3} D_v(\tilde{C} D_v \Psi_j)$$

where $M_r f_j = (f_{j+1/2} + f_{j-1/2})/2$. This is an example of an implicit time update belonging to the class of Keller-Preissman box schemes $[11]$. When expanded, the l.h.s. of the equations reads $(\partial^2_\phi \psi_{j+1} + 2 \partial^2_\phi \psi_j + \partial^2_\phi \psi_{j-1})/4$. Which means that one cannot update the value of $\psi_j$ without the updated values of $\psi_{j \pm 1}$. Implicit time-
updates could arise if one considers non-diagonal terms of the inverse volume operator [4, 13, 14]. Although these non-diagonal terms are likely to only become relevant near the classical singularity.

An interesting observation is that Eq. (5) can be rewritten as

$$\partial^2_{\hat{\phi}} \Psi_j = \frac{3}{2} \kappa \hat{B}^{-1} D_v (\hat{C} D_v \Psi_j) + \left( \frac{\Delta v^2}{2} \right)^2 D_v^2 \partial^2_{\hat{\phi}} \Psi_j. \quad (6)$$

In the semi-classical regime, where $O(\Delta v^2)$ terms can be ignored, Eq. (6) exhibits the same explicit temporal update as the standard LQC equation. On the other hand, near the classical singularity, one could apply $D_v^2$ to Eq. (6) and use the resulting equation to eliminated, recursively, in the r.h.s of Eq. (6) the terms with $\partial^2_{\hat{\phi}} \Psi_j$ in favor of higher order, spatial finite difference terms. However, in order to arrive to an equation that completely avoids the bounce, one would have to include enough higher order terms, that are effectively equivalent to an implicit update.

To derive the dispersion relation and group velocity for the modified LQC difference equation, we concentrate on the principal of Eq. (6) and perform a time-Fourier transform. One obtains $-\omega^2 M^2 \Psi_j = c^2 D_v^2 \bar{\Psi}_j$ with $c = \sqrt{3\kappa/2} |v|$. After substitution of the plane-wave solution, the dispersion relation in this case takes the form

$$\Delta v \omega \frac{2}{2c} = \pm \tan \left( \Delta v \frac{k}{2c} \right). \quad (7)$$

From which the group velocity reads,

$$V_g = \pm c \sec^2 \left( \frac{\Delta v k}{2c} \right) = \pm c \left[ 1 + \left( \frac{\Delta v \omega}{2c} \right)^2 \right]. \quad (8)$$

Clearly this type of time-update does not have a bounce or turning point. The group velocity does not vanish for $|v| \neq 0$. The characteristics in this case are $v = \sqrt{v^2 + v_{\phi}^2} e^{j \sqrt{10}} - v_{\phi}^2 1/2$. At $v = 0$, the group velocity becomes infinite because $c = 0$.

Fig. 1 shows the dispersion relation at an arbitrary point $|v| \neq 0$ for the WDW equation (solid line), the LQC equation with explicit time-update (long dashed line) and the modified LQC equation with implicit time-update (short dashed line). The constants of integration were chosen so the three characteristics have the same starting point when evolved backwards in time.

Fig. 3 shows an example of the characteristics of the continuum WDW equation (solid line), the LQC equation with explicit time-update (long dashed line) and the modified LQC equation with implicit time-update (short dashed line). The constants of integration were chosen so the three characteristics have the same starting point when evolved backwards in time.

FIG. 1: Dispersion relation at an arbitrary point $|v| \neq 0$ for the WDW equation (solid line), the LQC equation with explicit time-update (long dashed line) and the modified LQC equation with implicit time-update (short dashed line).
FIG. 2: An example of characteristics of the continuum WDW equation (solid line), the LQC equation with explicit time-update (long dashed line) and the LQC equation with implicit time-update (short dashed line). Constants of integration were chosen so the three characteristics have the same starting point when evolved backwards in time.

coefficients, explicit time-updates will typically couple the left- and right-moving fundamental modes and trigger reflections at the point where the group velocity vanishes. Explicit time integrations in LQC are tied to having a diagonal Hamiltonian for models in which one uses a single matter field as internal time [16]. In addition, we have investigated ad hoc modifications to the standard LQC finite difference equation that avoid the big quantum bounce while preserving a deterministic evolution across the big-bang singularity. The changes focused on replacing the explicit time update with an implicit scheme. Our numerical experiments showed that a semi-classical state at late times can be evolved backwards in time and reach the classical singularity in a finite time. At that point, the state gets partially transmitted. An interesting implication of this result is the outcome from an evolution forward in time of a right-moving (increasing \( v \) direction) state initially at the “other side” of the classical singularity. When the state reaches the classical singularity, it will yield a reflected wavefunction that remains on the other side of the singularity and a transmitted wavefunction emerging across the classical big bang into the physical sector.

Our analysis and numerical experiments were aimed at investigating the features in LQC homogeneous models with a massless scalar field that are related to the occurrence of a bounce. A complementary investigation, based on effective perturbation theory around a free scalar model, can be found in [17]. From a general perspective, our findings agree for dynamics which allows wave packets to reach small scales. Additional studies are needed to investigate whether more complicated models involving the issue of time could introduce modification similar to those considered here, in particular instances in which the LQC difference equation includes non-diagonal elements of the inverse volume operator. Those terms could have the potential of playing an important role near the big-bang singularity, significantly modifying or even preventing the big quantum bounce.

Acknowledgments

Thanks to A. Ashtekar, M. Bojowald, J. Hartle, D. Marolf, T. Pawlowski and P. Singh for helpful conversations, their comments and suggestions. This work was supported by NSF grants PHY-0244788 and PHY-0555436. CGWP is supported by the NSF under cooperative agreement PHY-0114375. Thanks also to the hospitality of KITP, supported by NSF PHY-9907949, where part of this work was completed.

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