No-boundary wave function for loop quantum cosmology

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Proposing smooth initial conditions is one of the most important tasks in quantum cosmology. On the other hand, the low-energy effective action, appearing in the semiclassical path integral, obtains nontrivial quantum corrections near classical singularities due to specific quantum gravity proposals. In this article, we combine the well-known no-boundary proposal for the wave function of the universe with quantum modifications coming from loop quantum cosmology (LQC). Remarkably, we find that the restriction of a "slow-roll" type potential in the original Hartle-Hawking proposal is considerably relaxed due to quantum geometry regularizations. Interestingly, the same effects responsible for singularity resolution in LQC also end up expanding the allowed space of smooth initial conditions leading to an inflationary universe.

I. MOTIVATION

Any theory of quantum cosmology must provide dynamical equations for the wave function of the universe as well as suitable boundary conditions for it. A well-known example for such a boundary condition is due to Hartle and Hawking (HH) [1],

$$\Psi^{\mathrm{HH}}[h_{ab}, \chi] := \int^{(h,\chi)} \mathcal{D}[g]\mathcal{D}[\varphi] e^{-S_{\mathrm{E}}[g,\varphi]/\hbar}. \qquad (1)$$

HH defines an initial state for the universe such that the path integral is over Euclidean 4-metrics bounded only by the 3-metric h and the value of the matter field on this hypersurface, χ. Traditionally, the weighting factor is given by (Euclidean) Einstein gravity, coupled to matter fields φ.

Loop quantum cosmology (LQC), on the other hand, is the application of quantization techniques from loop quantum gravity (LQG) to minisuperspace cosmological settings [2]. In this setting, the low-energy effective action is complemented by quantum geometrical corrections [3]. Canonically, it replaces the usual Wheeler–de Witt differential equation by a "difference equation", of finite step size, due to a regularized Hamiltonian constraint. Obviously, difference equations also require boundary conditions to extract specific solutions. Thus, the question of a suitable initial state remains important even for LQC [4,5].

In simple models of LQC, one usually chooses a semiclassical (nearly Gaussian) state at late times, peaked about some classical trajectory, and evolves it backwards to derive a bouncing solution [7]. However, this does not imply a deterministic bounce, as is sometimes incorrectly assumed, since a large portion of the state space remains unexplored. While conclusions regarding singularity resolution due to bounded curvatures and energy densities can be somewhat generically established in LQC [2], the precise mechanism, naturally, remains intricately tied to the initial state one chooses. In this article, we show that the original HH proposal, adapted to LQC, can lead to exciting new possibilities for a nonsingular quantum completion of inflation, profoundly expanding the range of allowed initial values for the scalar field.

Our starting point will be the path integral formulation of LQC [8–10], with paths weighted not by the Einstein-Hilbert (EH) action, but by a different one due to quantum geometry effects [11]. However, in the (relatively) low-energy limit, below $\mathcal{O}(10^{-3})$ Planck density, this action very rapidly reduces to the standard EH one [7]. Requiring a no-boundary-like wave function results in two main findings for this scenario. First, this provides a (topological) principle of setting initial conditions in LQC which would become important in avoiding *ad hoc* choices while dealing with, say, cosmological perturbations. More importantly, the LQC "effective' action, appearing in the no-boundary wave function, leads to finite probabilities for Lorentzian histories corresponding to an extended parameter space for inflation, due to novel instantonic solutions which were nonexistent in the EH case.

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II. FORMALISM

In this article, we follow the original HH proposal (with the prescribed contour [13,14]), albeit corresponding to the LQC effective action and not the EH one, explicitly demonstrating the existence of new saddle points which are different from the HH solution. Recently, it has been shown [15] that the Lorentzian path integral in EH quantum cosmology, analyzed using Picard-Lefshetz theory, does not have any contribution from the Euclidean saddle points proposed by HH (for a different perspective, see [16]). Although, in this work, we do not work with the Lorentzian path integral, this can easily be done for LQC and shall be pursued in future work.

On the LQC side, a technical gap we fill is to include nonperturbative expressions for "inverse-triad" modifications in the effective action appearing in the path integral. Previously, "holonomy modifications" were taken into account since they are primarily responsible for weighting the paths in a way so as to achieve singularity resolution [9]. However, we show that the inverse-triad corrections are essential for having well-defined (Euclidean) instantons, for a no-boundary-like wave function, near $a \to 0$. Rather remarkably, we find that due to these corrections, there exists solutions in scenarios where there were no well-defined instantons in the EH case, beyond the pure de-Sitter (dS) case.

The system under investigation is the closed FLRW cosmology $ds^2 = -N^2(t)dt^2 + a^2 d\Omega^2$, with Ω being the metric on a unit 3-sphere. For the $k = 1$ case, inverse-triad corrections are particularly relevant and provide significant modifications to LQC dynamics [17]. For the matter contribution (generically denoted by φ), we first choose to have only a positive cosmological constant Λ, and later a free scalar field ϕ. From now on, we use the convention that $\hbar = c = G = 1$.

Our no-boundary proposal for LQC (LQCNB) is given by

$$\Psi_{\rm NB}^{\rm LQC} = \int dN \int \mathcal{D}a\mathcal{D}\varphi\mathcal{D}p_\varphi\mathcal{D}p_a e^{-S_{\rm E}^{\rm LQC}}, \quad (2)$$

with the (Euclidean) LQC effective action, in its phase-space version ($\mathcal{H}^{\rm LQC}$ being the LQC Hamiltonian constraint), written as

$$S_{\rm E}^{\rm LQC} = \int_0^1 d\eta L_{\rm E} = \int d\eta(p_a\dot{a} - N\mathcal{H}_{\rm E}^{\rm LQC}). \quad (3)$$

One typically chooses the Euclidean time parameter to run from 0 to 1. However, following [18], we can introduce a parameter $\tau(\eta) := \int_0^\eta d\eta' N(\eta')$, such that one takes the integral over (complex) τ to go from τ_i to some τ_f. This is equivalent to choosing the proper time gauge by setting $N = 1$.

Since $\mathcal{H}_{\rm E}^{\rm LQC}$ is zero on shell, and the canonically conjugate momentum of the scale factor a is given by $p_a = -3\pi a\dot{a}/2$ [19], we can rewrite the action (on shell) as

$$S_{\rm E}^{\rm LQC} = -\frac{3\pi}{2}\int a\dot{a}^2 d\tau = -\frac{3\pi}{2}\int_0^{\tilde{a}} a\sqrt{|\mathcal{V}(a)|}da, \quad (4)$$

where $\dot{a}^2 = -\mathcal{V}(a)$. Note that this type of an equation, denoting a real Euclidean instanton as opposed to "fuzzy" complex instantons [18,20,21], can be obtained only for the specific choices of matter we make in this article—pure dS and a massless scalar field. In this form, the LQCNB can be written in the steepest descent approximation as

$$\Psi_{\rm NB}^{\rm LQC} \sim e^{-S_{\rm E}^{\rm LQC}[\tilde{a},\tilde{\varphi}]}, \quad (5)$$

where $\tilde{a} = a(\tau_f)$ [22]. By considering the effective Friedmann equation for such a model, one can calculate the $\mathcal{V}(a)$ required to completely evaluate this state.

III. PURE DE SITTER

Following [23], we can write the effective Friedmann equation (in $N = 1$ gauge) for $k = 1$ LQC as

$$-\dot{a}^2 = \mathcal{V} := \frac{8\pi a^2}{3}f^2(a)\left[\frac{\rho}{f(a)} - \rho_1\right]\left[\frac{\rho_2 - \frac{\rho}{f(a)}}{\rho_c}\right], \quad (6)$$

where

$$f(a) := \frac{1}{2}||v(a) - 1| - |v(a) + 1||, \quad (7)$$

$$\rho_1 := -\rho_c\left[\sin^2(\sqrt{\Delta}/a) - (1 + \gamma^2)\frac{\Delta}{a^2}\right], \quad (8)$$

$$\rho_2 := \rho_c\left[\cos^2(\sqrt{\Delta}/a) + (1 + \gamma^2)\frac{\Delta}{a^2}\right], \quad (9)$$

$$\rho := \frac{\Lambda}{8\pi}, \quad (10)$$

with the LQC critical density $\rho_c = \frac{3}{8\pi\gamma^2\Delta}$ and area gap $\Delta = 2\sqrt{3}\pi\gamma l_{\rm Pl}^2$, with γ being the Immirzi parameter. The dimensionless volume parameter $v(a)$ is related to the scale factor through the relation

$$v(a) = \left(\frac{6}{8\pi\gamma l_{\rm Pl}^2} \times (2\pi^2)^{2/3}\right)a^3. \quad (11)$$

It is sufficient to consider the (LQC) Friedmann equation in this case since the Raychaudhuri equation can be derived from it via a derivative with respect to τ. There are two regions in which the behavior of this equation is of interest to us. One is when we are near the $a \approx 0$ case. Note that one
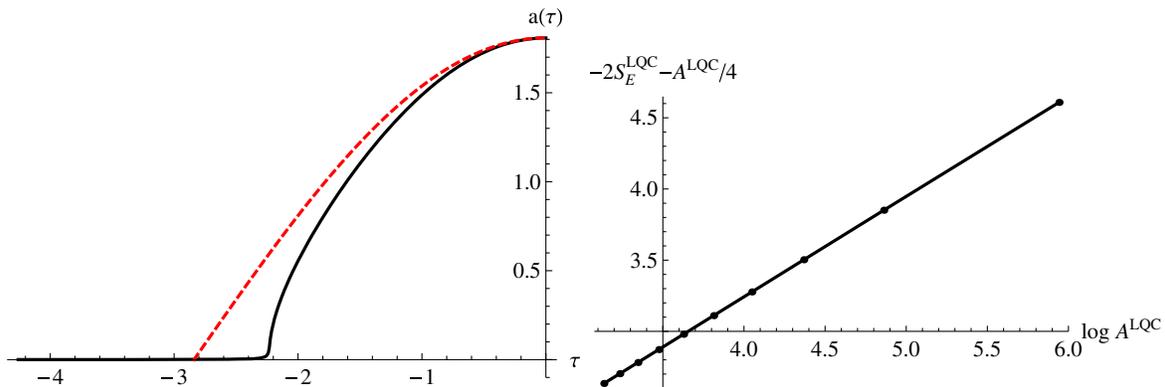
FIG. 1.   Left panel: A typical solution $a(\tau)$ for $\Lambda = 1$ and $l_{\text{Pl}} = 0.1$. The red dashed curve is the Einstein gravity case with the same $\tilde{a}$. Right panel: $-2S_E - \mathcal{A}/4$ versus $\log \mathcal{A}$. This shows Eq. (12).

never reaches this limit in the Lorentzian regime, and one concludes that there is a bounce, considering only Lorentzian histories. However, in order to investigate whether there is a well-defined, nonsingular instantonic solution to the Euclidean equations of motion, one needs to examine this limit. For $a \ll 1$, $f(a) \sim a^3$, whereas for $a \gg 1$, $f(a) = 1$. Thus, in the (relatively) large volume limit, we get the usual holonomy-modified LQC Friedmann equation, whereas in the other limit, the inverse-triad corrections play a crucial role to make the instanton nonsingular.

The integral defined in Eqs. (2) and (4), together with Eq. (6), is taken over a class of paths satisfying the final condition $a(\eta_f) = \tilde{a}$ and the initial condition $a(\tau_i) = 0$. For the HH initial state with the EH action, one further gets that $\dot{a}(\tau_i) = 1$ from the Hamiltonian constraint. However, in our case of LQCNB, such an instanton does not exist. If we still want to choose $a(\tau_i) = 0$ (since we wish to have a "regular closed-off geometry"), we get from Eq. (6) that $\dot{a} = 0$ as well. Thus, we see that not only are the "inverse-triad" corrections [manifested by the functions $f(a)$ [24]] crucial for a nonsingular instanton in this case, but they also lead to a solution that is geometrically (quantitatively) different from the HH one (left of Fig. 1).

The structure of the effective potential, $\mathcal{V}$, is too complicated, due to LQC corrections, to evaluate these path integrals analytically, even in the saddle-point approximation. Instead, we integrate it numerically and express the Euclidean (LQC) action as

$$-2S_E^{\text{LQC}} \simeq \frac{\mathcal{A}}{4} + c + d \log \mathcal{A} + \cdots, \qquad (12)$$

where $\mathcal{A} = 4\pi\tilde{a}^2$ (right of Fig. 1). Expressing the semiclassical factor in the quantum mechanical amplitude as above, the nucleation probability is

$$\mathcal{P} \simeq e^{-2S_E^{\text{LQC}}}. \qquad (13)$$

The comparison of this probability with the original HH state, with the EH action, reveals additional corrections, with LQC-dependent parameters c and d (more details on numerical calculations can be found in [25]). Assuming that the other constants of nature (such as γ) stay the same, c can be absorbed away with a change in the normalization, whereas the true corrections to the EH result come from the presence of a positive d. This shows that, in LQC, one has a greater probability of having a nucleating dS space. However, similar corrections might also appear from next-to-leading order calculations of the decay rate, and perhaps the only unambiguous conclusion is that corrections from LQC are small in this case.

IV. FREE SCALAR FIELD

Having shown that there exists a (different) instantonic solution for the well-studied ($k = 1$) dS universe for LQC, we now find Euclidean instantons for matter given by a massless scalar field. For the EH action, there exists no such nontrivial instantonic solutions for the no-boundary wave function (in the absence of any scalar-field potential). But the situation is qualitatively different for LQC due to modifications to the equation of motion of the scalar field. Once again, we first write down the effective Friedmann equation for the system as $\dot{a}^2 = -\mathcal{V}(a)$, with

$$\mathcal{V} = \frac{8\pi G}{3} a^2 f^2(a) \left[\frac{a^6 \pi}{4\sqrt{3}\gamma^3 l_{\text{Pl}}^6} \left(\frac{\rho}{\rho_c}\right) \left(\frac{g(a)}{f(a)}\right) - \rho_1 \right]$$
$$\times \left[\frac{1}{\rho_c} \left(\rho_2 - \frac{a^6 \pi}{4\sqrt{3}\gamma^3 l_{\text{Pl}}^6} \left(\frac{\rho}{\rho_c}\right) \left(\frac{g(a)}{f(a)}\right) \right) \right], \qquad (14)$$

where

$$g(a) := \frac{27}{8} ||v(a) + 1|^{1/3} - |v(a) - 1|^{1/3}|^3, \qquad (15)$$

$$\rho := \frac{p_\phi^2}{(2\pi^2)^2 a^6}. \qquad (16)$$

However, in this case, the usual relation between the momenta of the scalar field and its time derivative is also modified as follows:

$$p_\phi = \left(\frac{8\pi\gamma l_{\mathrm{Pl}}^2}{6}\right)^{3/2} B^{-1}(a)\dot{\phi} \qquad (17)$$

where

$$B(a) = \frac{2\pi^2}{\sqrt{3}}\left(\frac{8}{27}\right)\left(\frac{6}{8\pi\gamma l_{\mathrm{Pl}}}\right)^{3/2} a^3 g(a). \qquad (18)$$

These inverse-triad corrections $[f(a), g(a), B(a)]$ ensure a modification to the scalar-field equation as well:

$$\ddot{\phi} - \left(\frac{\dot{B}(a)}{B(a)}\right)\dot{\phi} = 0, \qquad (19)$$

with the general solution given by $\dot{\phi} = \dot{\phi}_0 B$, with constant $\dot{\phi}_0$. Using these two equations, one can derive the Raychaudhuri equation as in GR, albeit the form of it gets modified due to LQG corrections.

Looking at the asymptotic behavior of the function $g(a)$ defined above, it is straightforward to show that in the large volume limit, one gets that $B \sim 1/a^3$, thereby leading to the usual scalar-field equation

$$\ddot{\phi} + 3H\dot{\phi} = 0, \qquad (20)$$

where $H := \dot{a}/a$ is the Hubble parameter. In this case, we get the classical solution, $\dot{\phi} \sim 1/a^3$. On the other hand, when $a \ll 1$, we find that the effects of inverse-triad corrections kick in, setting up an antifriction term (with an opposite sign), leading to a "superinflationary" era. In this case, the equation is of the form

$$\ddot{\phi} - 12H\dot{\phi} = 0, \qquad (21)$$

leading to the solution $\dot{\phi} \sim a^{12}$ in this regime. This is crucial for our purposes of getting a well-defined, nonsingular instanton in this case as well, thanks to these additional factors of the scale factor coming from the inverse-triad terms. As the scale factor approaches zero, we find the regular instantonic solution at $(a = 0, \dot{a} = 0)$ like in the dS case. Unlike in the EH theory, we thus get a *new* instantonic solution for the LQC no-boundary wave function for a free inflaton field, thereby not requiring an inflationary "slow-roll" type potential term any longer for a smooth beginning in the deep quantum regime.

We have not said anything thus far regarding the initial conditions for the scalar field corresponding to our LQCNB state. For the original HH proposal, in the EH case, one *requires* the condition such that $\dot{\phi} \to 0$ as $a \to 0$, for well-behaved instantons (in the presence of some scalar potential). However, in this LQCNB case, we are free to choose any value for $\dot{\phi}_0$. There are, of course, other reasonable restrictions which have to imposed, such as having a $p_\phi \gg \hbar$, so that the state remains semiclassical at late times. This condition is important for the validity of the effective Friedmann equation in LQC as well as our saddle-point approximation, and has been enforced in our numerical investigations. On this note, let us mention an important distinction in how the term "semiclassical" is used in the original HH proposal and in standard LQC. The semiclassical (saddle-point) approximation of the HH wave function is quite different from the semiclassical limit in the sense of sharply peaked states frequently used in the LQC literature. As such, the two should not be confused with each other, and a precise relation between these two limits is beyond the scope of this paper.

From the numerical solutions, it is possible to observe that the $\mathcal{V}(a)$ has zeros if $a(\tau)$ satisfies one of two equations:

$$\frac{4}{27\sqrt{3}}\frac{\dot{\phi}_0^2}{\rho_c^2}\frac{g(a)}{f(a)} = -\sin^2\left(\frac{\sqrt{\Delta}}{a}\right) + (1+\gamma^2)\frac{\Delta}{a^2}, \qquad (22)$$
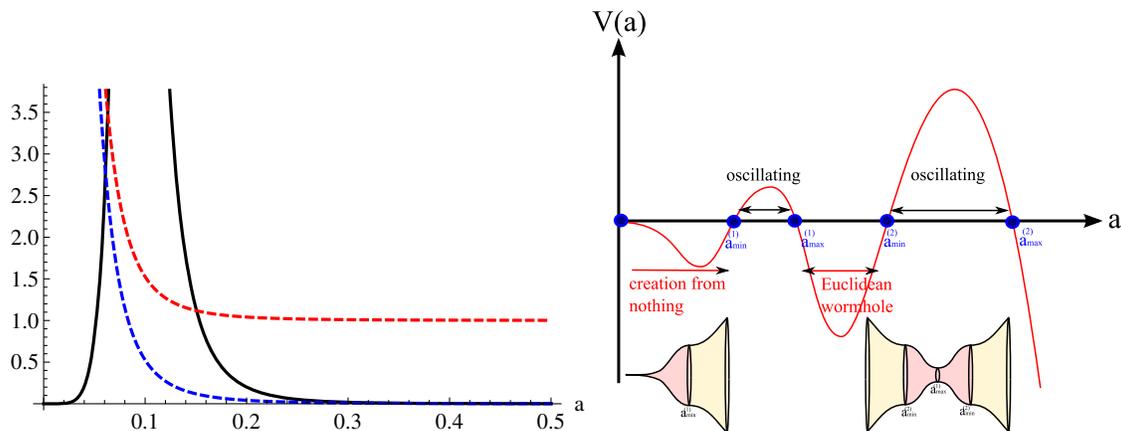

FIG. 2. Left panel: Left-hand sides of Eqs. (22) and (23) (black) and the right-hand sides of Eq. (22) (blue dashed) and Eq. (23) (red dashed) for $l_{\mathrm{Pl}} = 0.1$ and $\dot{\phi}_0 = 10^5$. This shows four zeros of $\mathcal{V}$ in Eq. (14). Right panel: A conceptual interpretation of $\mathcal{V}$.

$$\frac{4}{27\sqrt{3}}\frac{\dot{\phi}_0^2}{\rho_c^2}\frac{g(a)}{f(a)} = \cos^2\left(\frac{\sqrt{\Delta}}{a}\right) + (1+\gamma^2)\frac{\Delta}{a^2}. \quad (23)$$

On examining typical shapes, we see that there are four zeros in general, say, $0 < a_{\min}^{(2)} < a_{\max}^{(2)} < a_{\min}^{(1)} < a_{\max}^{(1)}$ (left of Fig. 2).

The usual interpretation in LQC for such models is that the universe oscillates between $a_{\min}^{(1)}$ and $a_{\max}^{(1)}$, two quantum bounces resolving the big bang and the big crunch singularities [23]. One does not consider oscillations between $a_{\min}^{(2)}$ and $a_{\max}^{(2)}$ since this region is usually assumed to be "forbidden" in LQC, if one considers only Lorentzian histories. However, now considering Euclidean trajectories, we get two possible scenarios (right of Fig. 2):

(1) The universe with size $a_{\min}^{(2)}$ is created from nothing. It begins oscillations between $a_{\min}^{(2)}$ and $a_{\max}^{(2)}$. At a certain time, the universe tunnels from $a_{\max}^{(2)}$ to $a_{\min}^{(1)}$. Eventually, it begins the second oscillation between $a_{\min}^{(1)}$ and $a_{\max}^{(1)}$, as is usually expected in LQC.

(2) Two universes with size $a_{\min}^{(1)}$ are created from nothing via a Euclidean wormhole [26,27], which starts from $a_{\min}^{(1)}$, decreases to $a_{\max}^{(2)}$, and bounces back to $a_{\min}^{(1)}$ via (real) Euclidean time.

V. CONCLUSION

One finds that LQC has a small contribution in the dS case but a substantially new result for the free scalar field. This is because in the former case, already in EH theory, there exists a potential barrier with a well-defined Euclidean instanton. Thus, LQC simply modifies the limits of this potential barrier for the universe to nucleate out of and results in a small correction to the EH result. In the free scalar field case, there exists no solutions to the (complex) equations of motion within the no-boundary proposal, for the EH case. However, for the LQCNB state, there exists a well-defined (real) Euclidean instanton even in the massless inflaton case, which corresponds to finite probabilities for a universe nucleating from nothing, or via a Euclidean wormhole.

The original no-boundary wave function was an attempt to formulate initial conditions for inflation as a topological principle; therefore, it is applicable to a variety of fundamental quantum gravity approaches. In this article, we show that such a "natural" initial condition [1], complemented by nonlocal (on the Planck scale) quantum geometry regularizations, results in a nonsingular quantum gravity extension for inflation, which is far more general than the original proposal. We find that there is an expanded range of initial conditions for the (momenta of the) inflaton field, allowing for a much larger class of potentials for setting up inflation. We study two extreme cases—pure dS and a massless inflaton field—with the latter being an example of new solutions for the no-

boundary wave function in LQC, having well-defined Euclidean saddle points where the EH theory did not. This opens up possibilities for a wide range of initial values, within the no-boundary proposal, leading to inflation due to necessary (loop) quantum gravity corrections to the EH action in deep quantum regimes. In other words, LQC corrections to the no-boundary proposal result in removing restrictions on the shape of the potential required for starting inflation, such as having a false vacuum. Furthermore, this would imply that the number of e-folds of inflation for LQCNB would be significantly different from the original EH case, due to the new freedom in choosing the initial velocity for the scalar field. This shall be investigated in future work.

On the LQC side, these types of proposals give us a new principle for choosing an initial state as well as a different way to understand singularity resolution. For instance, the universe could have been created from nothing in LQC, in addition to the usual bounce paradigm, with a natural interpretation of this as a superposition of histories with different probabilities. It is typically expected that the tunneling picture is subleading to the bounce exhibited by the effective trajectories for generic "sharply peaked" semiclassical states in LQC. [This is similar in spirit to the fact that the original HH wave function leads to a subdominant contribution as compared to the classical trajectories derived from (Lorentzian) Einstein's equations.] However, it is worth noting here that the new boundary conditions due to the no-boundary proposal may lead to different processes becoming dominant. A precise calculation comparing the probability of each of these events is not possible at the moment due to the requirement of relating the LQCNB wave function on the LQC Hilbert space with the so-called LQC semiclassical states, which is, as mentioned earlier, beyond the scope of this paper.

As an added feature, we find that the no-boundary state uncovers new physical phenomena in the Planckian era, such as the (Lorentzian) region between $a_{\min}^{(2)}$ and $a_{\max}^{(2)}$ in the free scalar field case. In this case, one can even consider scenarios with two arrows of time leading to rich possibilities for quantum cosmology. As we have shown, such a choice for smooth initial conditions is consistent with the conclusions for LQC background evolution at times soon after the "creation" of the universe, both in the dS and in the free scalar field case. Given this principle for choosing the initial state, one can perhaps distinguish between the different interpretations mentioned above by going beyond homogeneous minisuperspace backgrounds, which we set aside for future investigation.

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