Loop quantum gravity, signature change, and the no-boundary proposal

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Covariant models of loop quantum gravity generically imply dynamical signature change at high density. This article presents detailed derivations that show the fruitful interplay of this new kind of signature change with wave-function proposals of quantum cosmology, such as the no-boundary and tunneling proposals. In particular, instabilities of inhomogeneous perturbations found in a Lorentzian path-integral treatment are naturally cured. Importantly, dynamical signature change does not require Planckian densities when off-shell instantons are relevant.

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I. INTRODUCTION

The no-boundary proposal [1] shares with models of loop quantum gravity [2–4] a prominent role played by signature change. It is therefore of interest to discuss crucial technical differences but also unexpected synergies between these two approaches.

A general difference is given by how signature change features in these approaches to quantum cosmology—as a postulate in the no-boundary proposal and as an unexpected, derived result in models of loop quantum cosmology. The no-boundary proposal, in its simplest form with only a cosmological constant as the energy ingredient, implements specific initial conditions for the wave function of a universe by closing off an expanding Lorentzian space-time with a compact Euclidean cap at the big bang. Euclidean signature is introduced because it makes it possible to have 4-spherelike solutions that can provide such a closing cap. Here, signature change happens in a discontinuous manner by gluing together two semiclassical geometries with different signatures.

Models of loop quantum cosmology, by contrast, do not include Euclidean signature in their setup but rather derive, after what usually amounts to a long analysis, a modified space-time structure from other quantum effects in the dynamical equations that define such models. As one generic outcome, models of loop quantum cosmology may exhibit space-time structures with nonsingular signature change mediated by a curvature-dependent function that crosses zero in a continuous manner. For the sake of clarity, we will refer to the version of signature change realized in models of loop quantum gravity as *dynamical signature change*.

Another difference is that the no-boundary proposal contains signature change in the form of imaginary time, or a Wick rotation used in a Euclidean path integral, while models of loop quantum gravity work with real proper time. The reference to imaginary time in the no-boundary proposal can be eliminated by formulating it in a Lorentzian, as opposed to Euclidean, path integral [5,6], suggesting a potentially more direct correspondence with models of loop quantum gravity. However, in this case the no-boundary proposal is defined for off-shell instantons that solve the Raychaudhuri equation but not the Friedmann equation in order to implement the no-boundary initial condition of zero scale factor. In loop quantum cosmology, by contrast, the usual derivation of signature change requires certain identities that follow from a modified Friedmann equation (or its extension to inhomogeneous modes) and seem unavailable if only the Raychaudhuri equation is used.

On a more physical level, the no-boundary proposal works at sub-Planckian densities, assuming a small cosmological constant as the main source of stress-energy of a young universe. This is in fact one of its appealing features because it makes the proposal insensitive to detailed properties of quantum gravity. In models of loop quantum gravity, by contrast, signature change as discussed so far happens very close to Planckian densities. It relies on certain effects of loop quantum gravity not realized in classical general relativity, where signature change would be singular [7–10].

Given these discrepancies, an application of loop quantum gravity to the no-boundary proposal might seem useless. However, the relationship turns out to be closer than it appears at first sight, and it is actually fruitful: An application of the Lorentzian path integral to formulate the no-boundary proposal eliminates imaginary time giving the initial state of the universe a more physical interpretation.

But a new problem then arises because inhomogeneous perturbations around no-boundary instantons have been found to be unstable [11,12]. This result endangers the proposal as a well-defined initial scenario of the universe.

Unexpectedly, however, several properties of dynamical signature change in models of loop quantum cosmology conspire to solve the stability problem of the no-boundary proposal [13]. In the present paper, we highlight the details of several new properties of signature change for off-shell instantons in models of loop quantum gravity that are relevant for this conclusion. Importantly, this new version of dynamical signature change does not require Planckian densities, even though it is derived from the same loop-inspired modifications that lead to Planckian dynamical signature change in models *not* based on the no-boundary condition. On a technical level, our main results are therefore that (i) dynamical signature change can be derived for off-shell instantons in models of loop quantum gravity and (ii) can have markedly different features in this setting compared with on-shell solutions of modified constraint equations. We expand on our previous work [13] to give details of the saddle-point analysis and the structure of our new off-shell instantons. Moreover, we generalize our system to include and parametrize different quantization ambiguities associated with loop quantum gravity. We also point out several subtleties in the detailed derivation given here, which may be technical but are nevertheless surprising and essential for our physical results.

II. INSTABILITIES IN THE LORENTZIAN PATH INTEGRAL

We begin with a brief review of the Lorentzian path integral, following [5,6]. Boundary conditions for the no-boundary proposal can be formulated in a Lorentzian path integral of the usual integrand $\exp(iS/\hbar)$, as opposed to the Euclidean path integral of $\exp(-S/\hbar)$. Such an integral of a phase factor over real configurations usually converges very slowly, but convergence can be improved by an application of Picard–Lefshetz theory, shifting the integration contour onto the complex plane. Because the value of the integral is not changed thanks to Cauchy's theorem, provided the action S does not introduce poles in the complex plane, it remains Lorentzian even though complex configuration variables appear in the improved integration. It is therefore possible to avoid the use of imaginary time, and the original Lorentzian value of the path integral remains unmodified.

Preparing for an application of Picard–Lefshetz theory, the Lorentzian formulation of the no-boundary proposal deals with the problem of time by fixing time reparameterization invariance almost completely, specifying that the lapse function equals $N(t) = M/a(t)$ with a positive constant (rather than time-dependent function) M. (The factor of $1/a$ is introduced for convenience, and for the same reason transformed to the new variable $q = a^2$ [11,12].) Only this *constant* M, rather than a time-dependent function $N(t)$, is integrated over in path integrals. Because there is no longer a free multiplier at any given time, integration over M does not impose the Hamiltonian constraint or the Friedmann equation except at one time, which can be chosen to be the final moment included in a given path integral. This is the reason why path integrals in this formulation describe off-shell instantons, as a consequence of a specific approach to the problem of time.

A no-boundary instanton is then defined by the initial condition $q(0) = 0$, together with some fixed value of $q(1) = q_1$. For small t, a linear function $q(t) = q_1 t$ can be seen to solve the Raychaudhuri equation

$$\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} = 2\Lambda \tag{1}$$

for $q = a^2$ in the presence of a cosmological constant Λ (as well as positive spatial curvature). However, this initial condition cannot be compatible with the Friedmann equation for the same ingredients, given by

$$\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)^2 = 4(\Lambda q - 1). \tag{2}$$

The instantons considered in the Lorentzian formulation therefore must be strictly off-shell. (In the original Euclidean formulation, the condition $q = 0$ is compatible with the Wick-rotated version of (2).)

If the initial state is normalized, for simplicity assumed to be Gaussian, repeated path integrations over real configuration variables should preserve the Gaussian form. No instabilities could then arise. However, as it turns out, the equations of motion of inhomogeneous perturbations have solutions with branch cuts on the positive-M axis [12]. Picard–Lefshetz theory determines that this branch cut should be circumvented through the upper imaginary half-plane in the complex M-space. Along this contour, the action has a negative imaginary part, and the bounded $\exp(iS/\hbar)$ is turned into an unbounded upside-down Gaussian. Instabilities are then inevitable, a conclusion which refers to general properties of the space-time structure and also applies to alternative proposals of initial conditions, such as the tunneling proposal [14].

In more detail, the tensor mode equation for h in the time variable defined by choosing a lapse function $N = M/\sqrt{q}$, written conveniently for $v = qh$, is

$$\ddot{v} - \frac{\ddot{q}}{q} v - \frac{M^2}{q^2} \beta \nabla^2 v = 0 \tag{3}$$

where we include a parameter $\beta = \pm 1$ to see possible implications of space-time signature. For Lorentzian signature, $\beta = 1$, while $\beta = -1$ for Euclidean signature. In our subsequent application of methods of loop quantum cosmology, β will be a continuous function with $\beta \to 1$ at small curvature (late times).

For small t, the mode equation implies that

$$\ddot{v}_\ell \approx -\frac{\beta\ell(\ell+2)M^2}{q_1^2}\frac{v_\ell}{t^2} \tag{4}$$

for a fixed multipole number ℓ, solved by any superposition of the two independent solutions $v_{\ell,\pm} = t^{\frac{1}{2}(1\pm\gamma_\ell)}v_1$ where $v_1 = v(1)$ with

$$\gamma_\ell = \sqrt{1 - 4\beta\frac{\ell(\ell+2)M^2}{q_1^2}}. \tag{5}$$

The action for (4), derived from tensor modes restricted to leading terms at small t is

$$\begin{aligned} S_\ell &= \frac{1}{16\pi G}\int_0^1 \left(\frac{\dot{v}_\ell^2}{M} - \beta\ell(\ell+2)M\frac{v_\ell^2}{q^2}\right) \\ &= \frac{1}{16\pi GM}\int_0^1 \left(\dot{v}_\ell^2 + \frac{\gamma_\ell^2 - 1}{4t^2}v_\ell^2\right), \end{aligned} \tag{6}$$

inserting a small-t off-shell instanton with $q(t) = q_1 t$ in the second step. The appearance of M follows the characteristic dependence of matter or perturbation actions on the lapse function of a background metric.

Evaluated in $v_{\ell,\pm}$, we have

$$S_{\ell,\pm} = \frac{1}{32\pi GM}(1\pm\gamma_\ell)t^{\pm\gamma_\ell}|_{t=0}^1 v_1^2. \tag{7}$$

Only $v_{\ell,+}$ leads to a finite action $S_{\ell,+}$ because $\gamma_\ell > 0$; we therefore discard $v_{\ell,-}$. For complex M in the upper half plane, as dictated by Picard–Lefshetz theory,

$$S_{\ell,+} \propto \frac{1}{M} = \frac{\mathrm{Re}M - i\mathrm{Im}M}{|M|^2} \tag{8}$$

has a negative imaginary part which implies an unbounded $\exp(iS/\hbar)$.

Through γ_ℓ, the solutions $v_{\ell,\pm}$ have a branch cut at positive M for $\beta > 0$, in particular for $\beta = 1$ as used in the Lorentzian path-integral version of the no-boundary proposal. However, we can already see that any dynamical signature change that would turn β to negative values at small t can resolve the problem: If this happens, there is no branch cut on the real M-axis. An imaginary action and the corresponding instability could then be avoided. However, unlike in models of loop quantum gravity used so far, this dynamical signature change should happen (i) for off-shell instantons and (ii) at sub-Planckian curvature determined by a small cosmological constant. Each of these two conditions requires a detailed analysis.

III. OFF-SHELL INSTANTONS IN MODELS OF LOOP QUANTUM GRAVITY

In models of loop quantum gravity, the Hamiltonian constraint is modified by different effects motivated by mathematical properties of discrete space, most importantly inverse-triad corrections [15] and holonomy modifications [16]. Holonomy modifications are used to describe implications of the fact that loop quantum gravity implements operators not for the gravitational connection A_a^i (or extrinsic curvature K_a^i) but only for its SU(2)-holonomies in space [17,18]. Holonomies are based on parallel transport,

$$h_e = \mathcal{P}\exp\int_e A_a^i\tau_i\dot{e}^a \mathrm{d}\lambda, \tag{9}$$

and are therefore integrated over spatial curves e (with path ordering $\mathcal{P}$ of the noncommuting su(2) generators τ_i). As functions of the gravitational connection A_a^i, they are nonlinear and nonlocal.

In a homogeneous cosmological model, nonlocality in space is not visible because a position-independent connection then appears just as a collection of spatial constants in the exponent of (9). If the model is isotropic, for instance, any connection with positive spatial curvature can be expressed as $A_a^i = (\frac{1}{2}+c)\delta_a^i$ with a single canonical degree of freedom $c = \dot{a}$ [19], using a basis adapted to the symmetry. This degree of freedom is closely related to extrinsic curvature, $K_a^i = c\delta_a^i$, which is more convenient in setting up a class of states used in what follows [20,21]. Up to a constant phase factor, holonomies along integral curves of the symmetry generators, taken in an irreducible spin-j matrix representation of SU(2), then have matrix elements of the form $M_e = \exp(ij\ell_0\mu' c)$ with real numbers $-1 \le \mu' \le 1$. The fixed parameter ℓ_0 determines the coordinate size of a region in space which is taken as representative of the entire homogeneous geometry. (This region may but need not be the entire space. Nevertheless, to be specific, it can be taken to equal $\ell_0 = \sqrt[3]{2\pi^2}$ in the closed model.) The variable μ' then determines the length of the curve as a fraction of the reference length ℓ_0. Combining μ' with j, any real number $\mu = j\mu'$ can be achieved as a coefficient in the exponent of

$$M_\mu = \exp(i\ell_0\mu c). \tag{10}$$

A. Isotropic loop quantum cosmology

In a reduction of the symplectic structure of general relativity to isotropic models, c is seen to be canonically conjugate to a momentum $p \propto a^2$, such that

$$\{c, p\} = \frac{8\pi G}{3\ell_0^3}. \tag{11}$$

Alternatively, because $\ell_0 c$ automatically appears in matrix elements of holonomies, we may view $\ell_0 c$ and $\ell_0^2 p$ as canonical variables with a Poisson bracket independent of ℓ_0.

1. Representation

We use the Poisson structure to set up a canonical quantization [19,22], modeling properties of holonomies as operators in loop quantum gravity [17,18]. In this theory, a holonomy function (10) represents a normalizable state, unlike what would usually be the case in the standard representation of a canonical bracket (11). Loop quantization therefore exploits the existence of an inequivalent representation of (11) that exists if one does not require a quantization of (10) as a basic operator to be continuous in μ; see for instance [23].

This representation can be constructed by acting on the nonseparable Hilbert space of almost-periodic functions of c, defined as the space of functions linearly generated by the basis (10) for all real μ with inner product

$$\langle M_{\mu_1}, M_{\mu_2}\rangle = \lim_{C\to\infty} \frac{1}{2C}\int_{-C}^{C} M^*_{\mu_1}(c) M_{\mu_2}(c)\mathrm{d}c. \quad (12)$$

The momentum $\ell_0^2 p$ acts on the basis states via

$$\begin{aligned}\ell_0^2 \hat{p} M_\mu &= \frac{8\pi G\hbar}{3}\frac{\mathrm{d}}{i\,\mathrm{d}(\ell_0 c)}\exp(i\ell_0\mu c)\\ &= \frac{8\pi}{3}\ell_{\mathrm{P}}^2 \mu M_\mu = \ell_0^2 p_\mu M_\mu. \end{aligned} \quad (13)$$

The spectrum of $\ell_0^2\hat{p}/\ell_{\mathrm{P}}^2$ therefore contains all real numbers

$$\frac{p_\mu}{\ell_{\mathrm{P}}^2} = \frac{8\pi}{3}\mu, \quad (14)$$

but it is discrete because the eigenstates M_μ are normalizable. (These two properties are compatible with each other because the Hilbert space is nonseparable.)

To summarize, the nonlinearity of holonomies is implemented through the use of almost-periodic functions as states, on which the action of $\hat{M}_\mu$,

$$\hat{M}_{\mu_1} M_{\mu_2} = M_{\mu_1+\mu_2}, \quad (15)$$

is not weakly continuous at $\mu_1 = 0$. (In the Hilbert space used here, any two basis states, M_{μ_2} and $M_{\mu_1+\mu_2}$, are orthogonal for any $\mu_1 \neq 0$.) Therefore, it is not possible to derive a quantization of the linear phase-space function c by taking a derivative of M_μ at $\mu = 0$. Only the nonlinear functions $M_\mu(c)$ are represented as basic operators in addition to $\hat{p}$, which have to be used to construct possible quantizations of the polynomial Hamiltonian constraint (the Friedmann equation) of a cosmological model.

By replacing any polynomial reference to $c = \dot{a}$ in a classical expression by periodic functions, holonomy modifications are introduced. There is much freedom in choosing a periodic function to replace a polynomial, with the only condition that the classical polynomial should be obtained as an approximation for small c (or some other function of c being small, representing curvature). A common choice is to replace c in the Friedmann equation with $\sin(\ell(a)c)/\ell(a)$, where $\ell(a)$ is interpreted as a function that describes quantization ambiguities as well as properties of an underlying discrete state. In particular, the common choice $\ell(a) \approx \ell_{\mathrm{P}}/a$ with the Planck length ℓ_{P} [24] leads to corrections in the Friedmann equation that can be expanded in the dimensionless product $\ell_{\mathrm{P}}^2 H^2$ with the Hubble parameter H. Such corrections are relevant only near Planckian curvature.

2. Inverse-a corrections

The momentum operator $\hat{p}$ is represented directly as a basic operator. Moreover, it has all real numbers as eigenvalues, such that one could expect discretization effects to be minimal even though the spectrum is formally discrete. However, the discreteness can lead to significant quantum corrections whenever an inverse of p is quantized. Because $\hat{p}$ has a discrete spectrum containing zero, it does not have a densely defined inverse operator. Nevertheless, we need to quantize inverse powers of a or p that appear in the Hamiltonian constraint, for instance in the matter energy.

Using methods of [25], it is possible to construct densely defined operators such that their classical limits reproduce the required inverse power of a. The construction of these operators exploits the existence of commutator identities such as

$$\hat{M}_\mu^{-1}[\hat{M}_\mu, \ell_0\sqrt{\hat{p}}] = -\frac{4\pi}{3\ell_0}\ell_{\mathrm{P}}^2 \mu \widehat{p^{-1/2}}. \quad (16)$$

On the left-hand side, all operators are densely defined on the Hilbert space (taking the square root of $\hat{p}$ through the spectrum), and according to the right-hand side their combination quantizes an expression with classical limit proportional to $1/a$. An explicit calculation shows that the classical limit is well approximated when the commutator acts on a state M_{μ_2} with $\mu_2 \gg \mu$. For small $\mu_2 < \mu$, the behavior deviates from the classical limit, implying inverse-a corrections as a consequence of discrete spatial geometry [15].

As with holonomy modifications, the representation of a given inverse power of a as an operator via commutator identities is not unique, leading to additional quantization ambiguities. A detailed analysis of eigenvalues shows that inverse-a corrections can be parametrized broadly by a function $f(a)$, such that [26,27]

$$(a^{-1})_\mu = \frac{1}{a_\mu} f(a_\mu) \tag{17}$$

where a_μ is obtained by taking the square root of a $\hat{p}$-eigenvalue p_μ in (13). For large eigenvalues, $f(a_\mu) \sim 1$, while the small-μ behavior is a power law $f(a_\mu) \approx a_\mu^{2n}$ with a positive integer $n > 1$.

Holonomy modifications and inverse-a corrections result from modeling quantum-geometry effects of loop quantum gravity in isotropic situations. As always in an interacting theory, quantum corrections also arise from quantum backreaction of fluctuations and higher moments of a state on the expectation values [28,29]. Here, in accordance with the idea that the no-boundary proposal can describe the origin of space-time without strong quantum effects, we are interested in regimes in which quantum backreaction is subdominant compared with geometrical effects.

We will therefore analyze modified Friedmann equations in which inverse-a corrections have been inserted, mainly in the curvature and matter terms, and holonomy modifications have been used. For the latter, to be specific we will work with a function $\sin(\ell(a)c)/\ell(a)$ where the a-dependence of $\ell(a)$ is of power-law form, $\ell(a) = \ell_0\delta(\ell_0 a)^{2x}$ with constants δ (scaling like ℓ_0^{-1-2x}) and x. The exponent x is a parameter in an effective description and may therefore be running, such that it may take different values in different ranges of a curvature scale [30,31]. We will be able to ignore the running because our main results apply asymptotically close to the initial state of the no-boundary proposal. We will, however, take into account the possibility of having different constant values of x, depending on the theory and the underlying quantum-gravity state. As we will review in more detail later on, when the distinction will become important, two common choices for x are $x = 0$ (a constant co-moving length $\ell(a)$) and $x = -1/2$ (a constant geometrical length $a\ell(a)$).

3. Modified background dynamics

If ℓ depends on a in power-law form, it is convenient to introduce canonical variables such that $\ell(a)c$ is proportional to the new momentum:

$$Q = \frac{3(\ell_0 a)^{2(1-x)}}{8\pi G(1-x)} \quad \text{and} \quad P = -\ell_0^{2x+1} a^{2x}\dot{a}. \tag{18}$$

Moreover, we will use the definition $\bar{Q} = \frac{8}{3}\pi G(1-x)Q = (\ell_0 a)^{2(1-x)}$ in order to obtain more compact equations. In these variables, the classical constraint

$$C_{\rm class} = \ell_0^3\left(-\frac{3}{8\pi G}a(\dot{a}^2 + k) + a^3\rho\right) = 0, \tag{19}$$

is modified to

$$C = \frac{-3}{8\pi G}\left(\bar{Q}^{(1-4x)/(2(1-x))}\frac{\sin^2(\delta P)}{\delta^2} + \bar{Q}^{1/(2(1-x))}\kappa(Q)\right) + m(Q)g(Q) = 0 \tag{20}$$

with inverse-a corrections in the curvature term, $\kappa(Q)$, and in the matter term, $g(Q)$ multiplying the matter energy $m = \ell_0^3 a^3\rho$ contained in the averaging region of a homogeneous model. Classically, $g(Q) = 1$ while $\kappa(Q) = \ell_0^2$ for positive spatial curvature. In (19), we have included a factor of the coordinate volume ℓ_0^3 since the Hamiltonian constraint is spatially integrated.

Because the curvature term and the matter term depend on a through different powers, $\kappa(Q) \neq g(Q)$ in general. It is also possible that the P-dependent term in (20) is modified not just by holonomies (nonzero δ) but also by inverse-a corrections. Such a term may be required if there are explicit inverse powers of Q in (20), or if one extends the isotropic models used here to anisotropic ones, in which case even the classical constraint will have additional inverse powers of the anisotropic scale factors [21]. For now, we do not include such corrections in order to keep our equations reasonably short, noting that they can always be absorbed in the lapse function at the expense of further modifying $\kappa(Q)$ and $g(Q)$. Appendix A demonstrates that a modified lapse function that takes into account inverse-a corrections in the P-dependent term would not change our main results.

Canonical equations generated by C determine how P is related to $\dot{Q} = \{Q, NC\}$ for a given lapse function N. Upon evaluating this relationship, inverting it for P as a function of $\dot{Q}$, and inserting this expression in C, we obtain the modified Friedmann equation [32]

$$\left(\frac{\dot{a}}{Na}\right)^2 = \frac{8\pi G}{3}\left(\frac{m(a)}{\ell_0^3 a^3}g(a) - \frac{3}{8\pi G}\frac{\kappa(a)}{\ell_0^2 a^2}\right) \times \left(1 + \delta^2\frac{a^{4x}}{\ell_0^2}\kappa(a) - \frac{m(a)g(a)}{\ell_0^3 a^3\rho_{\rm QG}(a)}\right), \tag{21}$$

transformed back from Q to a, with a density scale

$$\rho_{\rm QG}(a) = \frac{3}{8\pi G\delta^2 a^{2(2x+1)}} \tag{22}$$

related to δ.

There is a single constraint in homogeneous models. Therefore, Hamilton's equations of motion $\dot{Q} = \{Q, NC\}$ and $\dot{P} = \{P, NC\}$ automatically preserve the constraint, for any lapse function N: $\dot{C} = \{C, NC\} = \{C, N\}C \approx 0$ vanishes when the constraint is satisfied. As a consequence, the Friedmann equation of a homogeneous model can easily be modified, as in (20), and then automatically generates consistent continuity and Raychaudhuri equations. However, it is not guaranteed that these evolution equations correspond to consistent evolution of an isotropic space-time setup as a background for a covariant theory of cosmological perturbations. (See [31,33] for a discussion of some subtleties in this context.) For isotropic models, it is sometimes possible [34–36] to construct analog actions which are covariant (of higher-curvature type) and produce modified Friedmann equations of the form (21). However, these actions fail to describe holonomy-modified equations of motion in anisotropic models [37] or for perturbative inhomogeneity [38].

4. Perturbation equations and covariance

The possibility of covariant perturbations on a modified background dynamics is therefore to be shown and cannot simply be assumed. In a canonical approach such as loop quantum gravity or its cosmological models, covariance can be tested systematically by an evaluation of Poisson brackets of constraints for perturbative inhomogeneity. Because inhomogeneous fields are subject to multiple constraints, consistency of their equations is not guaranteed: The Hamiltonian constraint $H[N(x)]$ and diffeomorphism constraint $D[M^a(x)]$ must be such that their Poisson brackets, which generically are not identically zero and even contain structure functions, vanish when the constraints are imposed. Moreover, for general covariance to be realized in the classical or low-curvature limit, their brackets must equal those of hypersurface deformations [39–41],

$$\{D[M_1^a], D[M_2^b]\} = D[\mathcal{L}_{M_1} M_2^c] \tag{23}$$

$$\{H[N], D[M^a]\} = -H[\mathcal{L}_{M_2} N] \tag{24}$$

$$\{H[N_1], H[N_2]\} = D[\beta q^{ab}(N_1\partial_b N_2 - N_2\partial_b N_1)], \tag{25}$$

in such a limit, where q^{ab} is the inverse spatial metric and $\beta = \pm 1$ determines space-time signature. If these brackets are closed after modifying the constraints, covariance remains intact but as a symmetry it may receive quantum corrections for instance in the structure function βq^{ab}.

Most modifications of holonomy form violate covariance [42], which can intuitively be seen from the fact that they only lead to corrections in terms of powers of $\dot{a}$, while covariant higher-curvature actions would also require higher time derivatives of a (or auxiliary fields). For specific modifications of the terms in an inhomogeneous constraint, it is possible to respect the closure condition of constraint brackets. However, the classical brackets are modified by a certain function

$$\beta(P) = \cos(2\delta P) \tag{26}$$

multiplying the bracket of two Hamiltonian constraints [43–45], assuming that the background Friedmann equation is modified according to (20). The modified theory therefore does not have gauge transformations of the classical form, which are equivalent to coordinate changes. Therefore, the form of covariance realized is not one of standard coordinate changes, at least not for the original metric variables. Nevertheless, under certain conditions it is possible to apply a field redefinition of the metric, such that the isotropic line element is not the usual canonical one,

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + a(t)^2\mathrm{d}\Omega_k, \tag{27}$$

but rather [46,47]

$$\mathrm{d}s_\beta^2 = -\beta N^2\mathrm{d}t^2 + a(t)^2\mathrm{d}\Omega_k. \tag{28}$$

When $\beta(P)$ is negative, the line element is positive definite, showing dynamical signature change. (In full generality, implications of these modified geometries for space-time structure are still being analyzed [48–50].) A modified constraint (20), together with trigonometric identities, implies that

$$\begin{aligned}\beta &= \cos(2\delta P) = 1 - 2\sin^2(\delta P) \\ &= 1 - 2\delta^2 \bar{Q}^{-(1-4x)/(2(1-x))} \\ &\quad \times \left(\frac{8\pi G}{3} m(Q) g(Q) - \bar{Q}^{1/(2(1-x))}\kappa(Q)\right) \\ &= 1 - 2\delta^2 a^{2(2x+1)}\left(\frac{8\pi G}{3}\rho g - \frac{\kappa}{a^2}\right) \\ &= 1 - 2\frac{\rho g}{\rho_{\mathrm{QG}}(a)} + \frac{3}{4\pi G}\frac{\kappa}{a^2 \rho_{\mathrm{QG}}(a)}\end{aligned} \tag{29}$$

where $\rho_{\mathrm{QG}}(a)$ has been defined in (22). If κ and g are such that the curvature term κ/a^2 is negligible compared with ρg at small a, we have $\beta < 0$ for $\rho g > \frac{1}{2}\rho_{\mathrm{QG}}(a)$. The usual choices of δ then require Planckian energy densities for signature change to be realized.

B. Off-shell instantons

The derivation of (29) requires an application of the Hamiltonian constraint (20) and is not available for off-shell instantons. As one of the main results reported in [13], it is nevertheless possible to derive β as a function of $\ddot{Q}$ instead of P. Unlike P, $\ddot{Q}$ is available for off-shell instantons because it is determined by the Raychaudhuri equation without reference to the Friedmann equation. Signature change is therefore a well-defined space-time phenomenon even for off-shell instantons, even though they do not satisfy all the equations implied by generators of hypersurface deformations. In the present paper, we demonstrate the nontrivial nature of this result.

However, we should first demonstrate the existence of off-shell instantons with no-boundary initial conditions, $q(0) = 0$ and $q(1) = q_1$, after a modification of background equations.

1. Existence

Off-shell Lorentzian instantons are determined by solving the second-order Raychaudhuri equation for the scale factor a or $q(=a^2)$ without imposing the first-order Friedmann equation. The usual matter choice in this context is a cosmological constant, $8\pi Gm/3\ell_0^3 = \Lambda a^3 = \Lambda q^{3/2}$. Since there is no inverse of a in such a matter term, $g(a) = 1$. Moreover, we follow [12] and choose the lapse function $N = M/a = M/\sqrt{q}$. We do not directly solve the modified Friedmann equation (21), or

$$\dot{q}^2 = -4M^2\left(\frac{\kappa(q)}{\ell_0^2} - \frac{1}{3}\Lambda q\right)\left(1 + \delta^2 q^{2x}\left(\frac{\kappa(q)}{\ell_0^2} - \frac{1}{3}\Lambda q\right)\right) \tag{30}$$

translated to q, but first take a second time derivative to obtain

$$\begin{aligned}\ddot{q} = {}& \frac{2}{3}\Lambda M^2\left(1 - \frac{3}{\Lambda\ell_0^2}\frac{\mathrm{d}\kappa}{\mathrm{d}q}\right)\left(1 + \delta^2 q^{2x}\left(\frac{\kappa(q)}{\ell_0^2} - \frac{1}{3}\Lambda q\right)\right)\\ & - 4x\delta^2 M^2 q^{2x-1}\left(\frac{\kappa(q)}{\ell_0^2} - \frac{1}{3}\Lambda q\right)\\ & \times\left(\frac{\kappa(q)}{\ell_0^2} - \frac{1}{6x}\Lambda\left(1 + 2x - \frac{3}{\Lambda\ell_0^2}\frac{\mathrm{d}\kappa}{\mathrm{d}q}\right)q\right).\end{aligned} \tag{31}$$

The right-hand side of (31) contains factors such as q^{-1} ($x = 0$) or q^{-2} ($x = -1/2$), but the full expression is nevertheless regular at $q = 0$ if inverse-q corrections are taken into account in $\kappa(q)$. The no-boundary initial value $q(0) = 0$ can therefore be imposed. For small t, q is small and the right-hand side of (31) is approximately constant. A generic small-t behavior of $q(t) \propto t + O(t^2)$ then follows.

It is not easy to find exact solutions of (31) for generic x and δ. As a simpler example, we may consider only inverse-triad corrections ($\delta = 0$), in which case the equation reads

$$\ddot{q} = \frac{2}{3}\Lambda M^2\left(1 - \frac{3}{\Lambda\ell_0^2}\frac{\mathrm{d}\kappa}{\mathrm{d}q}\right). \tag{32}$$

For large q, $\kappa \approx \ell_0^2$ and we recover the classical equation. For small q, $\kappa(q) \propto \ell_0^2 q^n$ is an integer power law in q, subject to quantization ambiguities. A simple analytical solution for $q(t)$ can be found if $\kappa(q) = \kappa_0\ell_0^2 q^2$ is quadratic, which implies

$$\begin{aligned}q(t) = {}& \left(q_1 + \frac{\Lambda}{6}(\cos(2\sqrt{\kappa_0}M) - 1)\right)\frac{\sin(2\sqrt{\kappa_0}Mt)}{\sin(2\sqrt{\kappa_0}M)}\\ & + \frac{\Lambda}{6}(1 - \cos(2\sqrt{\kappa_0}Mt))\end{aligned} \tag{33}$$

for no-boundary conditions $q(0) = 0$ and $q(1) = q_1$ as in [12]. A discussion of stability requires only the small-t behavior,

$$q(t) \approx \frac{2M\sqrt{\kappa_0}}{\sin(2\sqrt{\kappa_0}M)}\left(q_1 + \frac{\Lambda}{6}(\cos(2\sqrt{\kappa_0}M) - 1)\right)t + O(t^2). \tag{34}$$

As another example, holonomy modifications with $x = -1/2$ can be included if we assume an inverse-triad correction of the form $\kappa = \kappa_0\ell_0^2 q$. The equation of motion

$$\ddot{q} = 2M^2\frac{\Lambda}{3}\left(1 - \frac{3\kappa_0}{\Lambda}\right)\left(1 + \delta^2\left(\kappa_0 - \frac{\Lambda}{3}\right)\right) \tag{35}$$

then gives us a constant $\ddot{q}$, just as in the classical case, and is solved by

$$\begin{aligned}q(t) = {}& t^2 M^2\left(\frac{\Lambda}{3} - \kappa_0\right)\left(1 - \delta^2\left(\frac{\Lambda}{3} - \kappa_0\right)\right)\\ & + t\left(q_1 - M^2\left(\frac{\Lambda}{3} - \kappa_0\right)\left(1 - \delta^2\left(\frac{\Lambda}{3} - \kappa_0\right)\right)\right).\end{aligned} \tag{36}$$

2. Off-shell space-time structure

The analysis of hypersurface-deformation brackets in [44] determines β through the canonical momentum P. As indicated in (29), this expression can be written as a function of the energy density ρ upon using the modified Friedmann equation, but the latter is not available for off-shell instantons. We will now demonstrate that it is nevertheless possible to obtain a unique expression for β, based on the canonical version of the second-order equation for q. In order to capture potential quantization ambiguities based on the choice of basic variables that appear in holonomies, we work with the general expressions (18) for Q and P. The parameter x in P then determines the a-dependence of holonomy modifications. After P has been eliminated by inserting equations of motion, we will transform to the variable $q = a^2$ preferred for a comparison with the Lorentzian path integral.

We first derive the canonical version of modified equations of motion generated by (20), again following the choices of [12], in particular for the lapse function $N = M/a$. In this form, the constraint is given by

$$\begin{aligned}\frac{M}{a}C = {}& -\frac{3M\ell_0}{8\pi G}\left(\left(\frac{8\pi G}{3}(1-x)Q\right)^{-2x/(1-x)}\frac{\sin^2(\delta P)}{\delta^2}\right.\\ & \left. + \kappa(Q)\right) + M\frac{m(Q)g(Q)}{a(Q)}\end{aligned} \tag{37}$$

and generates first-order equations of motion

$$\begin{aligned}\dot{Q} &= \{Q, MC/a\}\\ &= -\frac{3M\ell_0}{8\pi G}\left(\frac{8\pi G}{3}(1-x)Q\right)^{-2x/(1-x)}\frac{\sin(2\delta P)}{\delta}\end{aligned} \tag{38}$$

$$\dot{P} = \{P, MC/a\} = \frac{3M\ell_0}{8\pi G}\left(-\frac{16\pi G x}{3}\left(\frac{8\pi G}{3}(1-x)Q\right)^{-(1+x)/(1-x)}\frac{\sin^2(\delta P)}{\delta^2} + \frac{\mathrm{d}\kappa}{\mathrm{d}Q}\right) - M\frac{\mathrm{d}(mg/a)}{\mathrm{d}Q}. \tag{39}$$

They imply the second-order equation

$$\begin{aligned}\ddot{Q} &= -\frac{3M\ell_0}{8\pi G}\left(-\frac{16\pi G x}{3}\left(\frac{8\pi G}{3}(1-x)Q\right)^{-(1+x)/(1-x)}\dot{Q}\frac{\sin(2\delta P)}{\delta} + 2\left(\frac{8\pi G}{3}(1-x)Q\right)^{-2x/(1-x)}\cos(2\delta P)\dot{P}\right)\\ &= 2\left(\frac{3M\ell_0}{8\pi G}\right)^2\left(\frac{8\pi G}{3}(1-x)Q\right)^{-2x/(1-x)}\left(\frac{8\pi G x}{3\delta^2}\left(\frac{8\pi G}{3}(1-x)Q\right)^{-(1+x)/(1-x)}(-\sin^2(2\delta P) + 2\sin^2(\delta P)\cos(2\delta P))\right.\\ &\quad\left. - \left(\frac{\mathrm{d}\kappa}{\mathrm{d}Q} - \frac{8\pi G}{3}\frac{\mathrm{d}(mg/(\ell_0 a))}{\mathrm{d}Q}\right)\cos(2\delta P)\right). \end{aligned}\tag{40}$$

Notice that this second-order equation is independent of (31) because it is derived from the phase-space expressions of equations of motion. As a second-order differential equation, it is not complete because it still contains P. The dynamics of q or Q is therefore determined by (31), and only by this equation in a consideration of off-shell instantons. Equation (40) then serves as an independent equation that can be used to determine $\cos(2\delta P)$, or β according to (26), as a function of $Q(t)$.

The trigonometric identity $\cos(2\delta P) = 1–2\sin^2(\delta P)$ allows us to simplify this expression to

$$\begin{aligned}\ddot{Q} = 2\left(\frac{3M\ell_0}{8\pi G}\right)^2\left(\frac{8\pi G}{3}(1-x)Q\right)^{-2x/(1-x)}&\left(\left(\frac{8\pi G x}{3\delta^2}\left(\frac{8\pi G}{3}(1-x)Q\right)^{-(1+x)/(1-x)}\right.\right.\\ &\left.\left. - \left(\frac{\mathrm{d}\kappa}{\mathrm{d}Q} - \frac{8\pi G}{3}\frac{\mathrm{d}(mg/(\ell_0 a))}{\mathrm{d}Q}\right)\right)\cos(2\delta P) - \frac{8\pi G x}{3\delta^2}\left(\frac{8\pi G}{3}(1-x)Q\right)^{-(1+x)/(1-x)}\right).\end{aligned}\tag{41}$$

Importantly, we have eliminated all quadratic terms in $\cos(2\delta P)$ or $\sin(2\delta P)$. Therefore, we can uniquely solve the equation for

$$\begin{aligned}\cos(2\delta P) &= \frac{\frac{8\pi G x}{3\delta^2}(\frac{8\pi G}{3}(1-x)Q)^{-(1+x)/(1-x)} + \frac{1}{2}\ddot{Q}(\frac{8\pi G}{3M\ell_0})^2(\frac{8\pi G}{3}(1-x)Q)^{2x/(1-x)}}{\frac{8\pi G x}{3\delta^2}(\frac{8\pi G}{3}(1-x)Q)^{-(1+x)/(1-x)} - \mathrm{d}\kappa/\mathrm{d}Q + \frac{8\pi G}{3}\mathrm{d}(mg/(\ell_0 a))/\mathrm{d}Q}\\ &= \begin{cases}\frac{1+\frac{4\pi G\delta^2}{3xM^2\ell_0^2}(\frac{8\pi G}{3}(1-x)Q)^{(1+3x)/(1-x)}\ddot{Q}}{1+\frac{\delta^2}{x}(\frac{8\pi G}{3}(1-x)Q)^{(1+x)/(1-x)}(\mathrm{d}(mg/(\ell_0 a))/\mathrm{d}Q - \frac{3}{8\pi G}\mathrm{d}\kappa/\mathrm{d}Q)} & \text{if } x \neq 0\\ \frac{\frac{1}{2}\ddot{Q}(\frac{8\pi G}{3M\ell_0})^2}{\frac{8\pi G}{3}\mathrm{d}(mg/(\ell_0 a))/\mathrm{d}Q - \mathrm{d}\kappa/\mathrm{d}Q} & \text{if } x = 0\end{cases}\end{aligned}\tag{42}$$

in terms of $\ddot{Q}$, without taking a square root.

Writing $\cos(2\delta P)$ suggests that there is still a P, which however is determined only by first-order equations that are not available for off-shell instantons. For off-shell instantons, we can instead use (42) as the only equation left in the system that determines P. The resulting value of P may not be real because the right-hand side of (42) is not restricted to be between one and -1. This possibility of imaginary P is the analog of an imaginary $\mathrm{d}q/\mathrm{d}t$ implied by the classical first-order equation (21) at the no-boundary initial time, where $q = 0$. As in this case, a complex P here is not problematic in a discussion of off-shell instantons.

What is important is that (42) uniquely determines $\cos(2\delta P)$ as a real function, even if P may not be real. This real function can be taken as a definition of β following (26) derived from the results of hypersurface-deformation brackets for perturbative inhomogeneity. These results use only the off-shell Poisson brackets of constraints for inhomogeneous perturbations and therefore remain available for off-shell instantons. We recall the important feature seen in the final equation (41), which is linear in $\cos(2\delta P) = \beta$, such that no roots need be taken that could limit the allowed range of values. (The intermediate step (40) demonstrates that this result is quite nontrivial.) This outcome is crucial for our extension of dynamical signature change in models of loop quantum cosmology to off-shell instantons.

At this point, it is convenient to apply the inverse transformation of (18) from Q to

$$q = a^2 = \frac{1}{\ell_0^2}\left(\frac{8\pi G}{3}(1-x)Q\right)^{1/(1-x)}. \tag{43}$$

Using

$$\frac{\mathrm{d}}{\mathrm{d}Q} = \frac{\mathrm{d}q}{\mathrm{d}Q}\frac{\mathrm{d}}{\mathrm{d}q} = \frac{8\pi G}{3}\ell_0^{2(x-1)}q^x\frac{\mathrm{d}}{\mathrm{d}q} \tag{44}$$

and

$$\ddot{Q} = \frac{3\ell_0^{2(1-x)}}{8\pi G}\left(\frac{\ddot{q}}{q^x} - x\frac{\dot{q}^2}{q^{1+x}}\right), \tag{45}$$

the resulting expression for the off-shell $\beta = \cos(2\delta P)$ is

$$\beta = \frac{1 + \frac{1}{2}M^{-2}\delta^2 x^{-1}\ell_0^{2(1+2x)}q^{1+2x}(\ddot{q} - x\dot{q}^2/q)}{1 + \delta^2 x^{-1}\ell_0^{4x}q^{1+2x}(\frac{8\pi G}{3}\mathrm{d}(mg/(\ell_0\sqrt{q}))/\mathrm{d}q - \mathrm{d}\kappa/\mathrm{d}q)} \tag{46}$$

for $x \neq 0$ and

$$\beta = \frac{\ell_0^2}{2M^2}\frac{\ddot{q}}{\frac{8\pi G}{3}\mathrm{d}(mg/(\ell_0\sqrt{q}))/\mathrm{d}q - \mathrm{d}\kappa/\mathrm{d}q} \tag{47}$$

for $x = 0$. (The expression for $x = 0$ is independent of δ but differs from the classical value one. The classical limit $\beta \to 1$ can be obtained from (42) if the limit $\delta \to 0$ is taken before $x \to 0$.)

3. Renormalization parameters

There are two common (but nonunique) choices for x: If $x = 0$, $Q = 3\ell_0^2 a^2/(8\pi G)$ is proportional to the isotropic version of a densitized triad, and $P = -\ell_0\dot{a}$ is the isotropic component of the connection or extrinsic curvature. These tensors are used as basic variables in loop quantum gravity. At a technical level, this case is therefore preferred in fundamental constructions. However, it implies a fixed comoving discreteness scale δ in the holonomy used to quantize the Hamiltonian constraint which can easily grow to macroscopic values as the universe expands: Writing the argument of holonomies in this case as $\delta P = -\delta\ell_0\dot{a} = -\delta\ell_0 aH$ shows that it can grow very large during an inflationary period with nearly constant Hubble parameter H.

Using a homogeneous cosmological model in considerations of long evolution times, in particular during inflation, means that one is applying an effective description of a fundamental theory on a vast range of scales. It is not reasonable to expect that the same effective theory, with constant parameters, remains valid over the whole range. Parameters that describe the effective dynamics should rather be adjusted, or renormalized, as the scales change. The averaging of a fundamental state implicitly described by a homogeneous minisuperspace model is therefore expected to lead to a running x as well as δ. The effective power-law exponent x may still describe the effective evolution in sufficiently short periods of time, but it need not be equal to zero or remain constant.

While the derivation of a running x from a fundamental discrete theory is challenging, it is possible to model possible outcomes of cosmic evolution by a succession of phases with different x, such that x is nearly constant in each phase (much like the energy density is usually assumed to be of power-law form depending on the dominant matter contribution). If $x < 0$, $P = -\ell_0^{2x+1}a^{2x}\dot{a}$ contains a suppression by the scale factor, such that the increase of the discreteness scale is slowed down compared with $x = 0$. For $x = -1/2$, we have $P = -H$, and the scale remains constant if H is constant. This value is therefore preferred from the perspective of model building *if* one assumes that a long period of cosmic evolution can be described without renormalization [51]. However, given the general expectation that renormalization does take place, the argument cannot be used to show that only the value $x = -1/2$ is possible [31].

New arguments that do not require long cosmic evolution are therefore necessary if one tries to restrict possible choices of x. An example is the observation made in [44] that the value $x = -1/2$ may be preferred in constructions of consistent holonomy modifications in the constraints for perturbative inhomogeneity. We are now ready to derive a new result of this form based on signature change in off-shell instantons. We therefore return to our Eqs. (46) and (47) for β depending on x, and recall that $\beta < 0$ is of advantage in the no-boundary proposal because it moves the branch cut of (5) from the real axis to the imaginary axis, eliminating the imaginary part of the action evaluated on no-boundary instantons.

First looking at the case of $x = 0$, Eq. (47) evaluated for small-t no-boundary solutions such that $q(t) \propto t$, we see that $\beta = 0$. While this value differs significantly from the classical behavior, it does not imply signature change with $\beta < 0$. For $x = -1/2$, assuming as usual that $8\pi Gm/3\ell_0^3 = \Lambda q^{3/2}$ is determined completely by a cosmological constant Λ and ignoring inverse-triad corrections ($g = 1$ and $\kappa/\ell_0^2 = 1$), we obtain

$$\beta = \frac{1 - (\delta/M)^2(\ddot{q} + \frac{1}{2}\dot{q}^2/q)}{1 - 2\delta^2\Lambda} \tag{48}$$

from (46). For sub-Planckian Λ, the denominator is close to one. For small-t no-boundary solutions, we have $q(t) \approx ct$ as shown in Sec. III B 1, such that

$$\beta \approx 1 - \frac{\delta^2 c}{2M^2}\frac{1}{t} < 0 \tag{49}$$

is negative as long as $t < \frac{1}{2}\delta^2 c/M^2$. Since we will now set out to demonstrate that this version of signature change is able to rescue the no-boundary proposal, we have obtained another reason why $x = -1/2$ should be preferred compared with $x = 0$, if only these two choices are considered. More generally, (46) evaluated on small-t off-shell instantons implies that

$$\beta = \frac{1 - \frac{1}{2}(M\ell_0)^{-2}\delta^2(\ell_0^2 c)^{2(1+x)}t^{2x}}{1 + x^{-1}\delta^2(\ell_0^2 c)^{1+2x}\Lambda t^{1+2x}} \qquad (50)$$

for any $x \neq 0$. For $x < -1/2$, both numerator and denominator may be negative for small t. The presence of signature change therefore depends on relationships between parameters such as Λ and δ, and is not as generic as in (49). The range $-1/2 < x < 0$ leads to a qualitative behavior similar to $x = -1/2$, but the phase of signature change becomes shorter and shorter as x approaches zero because the pole of t^{2x} in the numerator of β then weakens. The value $x = -1/2$ therefore optimizes the generic nature and duration of signature change, maximally stabilizing perturbations around off-shell instantons.

As just mentioned, the function (49) has a pole at $t = 0$, which will imply a subtlety in our detailed stability analysis given in the following subsection. When transforming (41) for $x = -1/2$ from Q to q using (44) and (45), we encounter the expression

$$\ddot{q} = -\frac{1}{2}\frac{\dot{q}^2}{q} + M^2\left(\frac{16\pi G}{3}\beta\frac{\mathrm{d}(q\rho)}{\mathrm{d}q} + \frac{1-\beta}{\delta^2}\right), \qquad (51)$$

evaluated here for $\kappa = \ell_0^2$ and $g = 1$, writing $\rho = m/\ell_0^3 a^3$. We can see that the pole of β has a direct relationship with the no-boundary initial condition, which implies that the left-hand side is zero while the pole of $-\frac{1}{2}\dot{q}^2/q = -\frac{1}{2}c/t$ in the first term on the right-hand side must be canceled if the equation holds true. The pole in β, which changes the asymptotic form of the mode equation (4), is therefore directly implied by the no-boundary initial condition.

4. Stability

Covariant equations compatible with (21) have been derived in [44], as well as in [43,52] for spherically symmetric models with closely related properties [45]. For small t and q, we assume, as before, that $g(q) = g_0 q^n$ is a power law with some integer n and positive $g_0 > 0$. Tensor perturbations $h(\eta)$ in conformal time η are then subject to [44]

$$h'' + \left(2(1+n)\frac{a'}{a} - \frac{\beta'}{\beta}\right)h' - \frac{\beta}{\Sigma}\nabla^2 h = 0 \qquad (52)$$

with

$$\Sigma = \frac{1}{g_0}\frac{2n-3}{(1+n)(n-3)}. \qquad (53)$$

Since n is an integer, $\Sigma > 0$ unless $n = 2$. From now on we will assume the generic case, $n \neq 2$ such that Σ is positive.

Again, we transform to $q = a^2$ instead of a and use a time coordinate according to $N = M/a$, obtaining

$$\ddot{v} - \left(\frac{\ddot{z}}{z} + \frac{\dot{\beta}^2}{4\beta^2} + \frac{\ddot{\beta}}{2\beta}\right)v + \frac{M^2}{q^2}\frac{\beta}{\Sigma}\nabla^2 v = 0 \qquad (54)$$

where $z = q^{1+n/2}/\sqrt{|\beta|}$ and $v = zh$. We first demonstrate how dynamical signature change can lead to stability by assuming that β is nearly constant and negative for some range of small q, which leads to an easy comparison with the results of [12]. For a tensor mode of multipole moment ℓ and an off-shell instanton (34), the small-t mode equation is then

$$\ddot{v}_\ell \approx \left(\frac{n(n+2)}{4} - \beta\frac{\ell(\ell+2)\sin^2(2\sqrt{\kappa_0}M)}{4\Sigma\kappa_0(q_1 + \frac{1}{6}\Lambda(\cos(2\sqrt{\kappa_0}M) - 1)^2)}\right)\frac{v_\ell}{t^2}$$
$$= \frac{\gamma_\ell^2 - 1}{4}\frac{v_\ell}{t^2}.$$

As in [12], there are two independent solutions $v_{\ell,\pm} = t^{\frac{1}{2}(1\pm\gamma_\ell)}v_1$, but γ_ℓ is modified. As an example, we can ignore inverse-a corrections by setting $n = 0$ and $2\sqrt{\kappa_0}M \ll 1$ in (34), and obtain

$$\gamma_\ell = \sqrt{1 - 4\beta\frac{\ell(\ell+2)M^2}{\Sigma q_1^2}}. \qquad (55)$$

The case of $\beta = 1$, used in [12], implies branch cuts on the real M-axis for both solutions $v_{\ell,\pm}$. The action for modes evaluated in these solutions, (7), then acquires imaginary parts that lead to instability. With effects from loop quantum cosmology, in particular dynamical signature change, we have $\beta < 0$ such that γ_ℓ does not have branch cuts on the real M-axis. Therefore, one does not expect unstable Gaussians to result from a path integration over M.

The full equation (55) also shows that inverse-a corrections can change the positions of branch cuts. Even if $\beta > 0$, inverse-a corrections can partially improve stability, but real γ_ℓ are then obtained only for a finite number of multipoles, with a maximum value related to the ambiguity parameter n. If we had only inverse-a corrections, models of loop quantum gravity would not lead to complete stability. Nevertheless, including inverse-a corrections in (55) is useful because it shows that they do not interfere with stability as implied by holonomy modifications when β is negative.

In the asymptotic regime of very small t, which is most relevant for no-boundary initial conditions, it is not possible to assume nearly constant β because (49) has a pole at $t = 0$. This pole, rather than the classical $1/t^2$-behavior, dominates the mode equation

$$\ddot{v}_\ell = \left(\frac{\ddot{z}}{z} + \frac{\dot{\beta}^2}{4\beta^2} + \frac{\ddot{\beta}}{2\beta}\right) v_\ell + \frac{M^2\ell(\ell+2)\beta}{q^2} \frac{\beta}{\Sigma} v_\ell \approx \frac{\alpha_\ell v_\ell}{t^3} \tag{56}$$

where $\alpha_\ell = \frac{1}{2}\delta^2\ell(\ell+2)/(\Sigma c) > 0$. This equation can be solved by modified Bessel functions of the second kind, and we obtain

$$v_\ell(t) = \sqrt{t}\frac{K_1(\sqrt{\alpha_\ell/t})}{K_1(\sqrt{\alpha_\ell})} v_1 \tag{57}$$

for the regular solution.

The action is now given by

$$S_\ell = \frac{1}{16\pi GM}\int_0^1 \left(\dot{v}_\ell^2 + \frac{\alpha_\ell}{4t^3} v_\ell^2\right) \mathrm{d}t. \tag{58}$$

It is convenient to integrate by parts,

$$S_\ell = \frac{1}{16\pi GM}(v_\ell \dot{v}_\ell)|_{t=0}^1 - \frac{1}{16\pi GM}\int_0^1 \left(v_\ell \ddot{v}_\ell - \frac{\alpha_\ell}{4t^3} v_\ell^2\right) \mathrm{d}t, \tag{59}$$

in which the last integral vanishes thanks to the mode equation. We can then simply insert the regular solution (57) in the boundary term and use $K_1'(z) = -K_0(z) - K_1(z)/z$:

$$S_\ell = \frac{1}{32\pi G}\frac{\sqrt{\alpha_\ell}}{K_1(\sqrt{\alpha_\ell})^2}\frac{K_1(\sqrt{\alpha_\ell/t})K_0(\sqrt{\alpha_\ell/t})}{\sqrt{t}}\bigg|_{t=0}^1 v_1^2. \tag{60}$$

The asymptotic behavior $K_j(z) \sim \sqrt{\pi/2z}e^{-z}$ for $z \gg j$ shows that the action

$$\begin{aligned} S_\ell &\sim \frac{\pi}{32\pi G K_1(\sqrt{\alpha_\ell})^2}\exp(-2\sqrt{\alpha_\ell/t})\bigg|_{t=0}^1 v_1^2 \\ &= \frac{\pi}{32\pi G K_1(\sqrt{\alpha_\ell})^2} v_1^2 \end{aligned} \tag{61}$$

is finite.

The function (49) implies signature change if and only if $\alpha_\ell > 0$ for all ℓ. The same condition results in a real action (61) without any imaginary part that could lead to instabilities, as in (7). Moreover, the leading asymptotic order in (56) is completely independent of M because the M-dependence of the spatial derivative term in the general mode equation cancels out with the M-dependence in (49). The action, therefore, does not have any branch cuts in the complex M-plane.

IV. CONCLUSIONS

Our detailed derivations of mode equations in the Lorentzian no-boundary proposal for loop quantum cosmology have revealed several subtle features which conspire to stabilize perturbative inhomogeneity around off-shell instantons with no-boundary conditions.[1] In particular, the possibility of sub-Planckian signature change in off-shell instantons is surprising and constitutes a new physical effect even though it is based on the same constraint analysis [44] as in the standard on-shell treatment in loop quantum cosmology. The precise form of the signature function (49) then showed several important features—related to its pole, the sign of its coefficients, and the dependence on the lapse function—that played important roles in our stabilization results. The constructive interplay between loop quantum cosmology and the no-boundary proposal (or any initial-value formulation in the Lorentzian path integral) is therefore highly nontrivial.

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APPENDIX A: INVERSE-a CORRECTIONS, ABSORBED IN THE LAPSE FUNCTION

If the P-dependent term in the Hamiltonian constraint (20) contains inverse-a corrections $\eta(Q)$, they can be absorbed in the lapse function provided $\kappa(Q)$ and $g(Q)$ are changed accordingly. For most of our calculations, we worked with general expressions for the latter two functions, but we assumed that $N = M/\sqrt{q}$ with constant M. If inverse-a corrections are absorbed in the lapse function, our equations will receive additional terms because the q-dependence of N changes. Here, we show that the resulting equations do not endanger our main result.

In the constraint and Friedmann equations, we can in this case simply replace N with $N\eta(Q)$, $\kappa(Q)$ with $\kappa(Q)/\eta(Q)$, and $g(Q)$ with $g(Q)/\eta(Q)$. Equation (21), for instance, will be multiplied by η^2 on the right, and (29) remains unchanged because it is obtained by setting the constraint equal to zero, such that any N or $N\eta$ cancel out.

However, new terms arise as soon as we start taking time derivatives of our initial equations. While (30) is just modified by using $M\eta$ instead of M, the term

$$-4M^2\eta\frac{\mathrm{d}\eta}{\mathrm{d}q}\left(\frac{\kappa}{\ell_0^2} - \frac{1}{3}\Lambda q\right)\left(1 + \delta^2 q^{2x}\left(\frac{\kappa}{\ell_0^2} - \frac{1}{3}\Lambda q\right)\right) \tag{A1}$$

[1] Without incorporating the crucial input of dynamical signature-change, one would not be able to see these features as has been noted in [53,54]. These studies rather focused on providing new insight on how the no-boundary wave function can reveal new interesting dynamics in models of loop quantum cosmology by setting up novel initial conditions.

must be added to (31). Therefore,

$$\ddot{q} = \frac{2}{3}M^2\eta^2\Lambda\left(1 - \frac{3}{\Lambda} + 2\frac{\mathrm{d}\log\eta}{\mathrm{d}\log q} - \frac{6\kappa}{\Lambda\ell_0^2}\frac{\mathrm{d}\log\eta}{\mathrm{d}q}\right)\left(1 + \delta^2 q^{2x}\left(\frac{\kappa(q)}{\ell_0^2} - \frac{1}{3}\Lambda q\right)\right) - 4x\delta^2 M^2\eta^2 q^{2x-1}\left(\frac{\kappa(q)}{\ell_0^2} - \frac{1}{3}\Lambda q\right)\left(\frac{\kappa(q)}{\ell_0^2} - \frac{1}{6x}\Lambda\left(1 + 2x - \frac{3}{\Lambda}\frac{\mathrm{d}\kappa}{\mathrm{d}q}\right)q\right). \tag{A2}$$

In (38), we again simply replace M with $M\eta$. In (39), we make the same replacement, but also add the term

$$\frac{3M\ell_0}{8\pi G}\frac{\mathrm{d}\eta}{\mathrm{d}q}\left(\left(\frac{8\pi G}{3}(1-x)Q\right)^{-2x/(1-x)}\frac{\sin^2(\delta P)}{\delta^2} + \kappa\right) - M\frac{mg}{\sqrt{Q}} \tag{A3}$$

implied by a Q-derivative of the constraint. The additional time derivative taken to derive (40) leads to further terms, such that now

$$\ddot{Q} = 2\left(\frac{3M\ell_0\eta}{8\pi G}\right)^2\left(\frac{8\pi G}{3}(1-x)Q\right)^{-2x/(1-x)}\left(\frac{8\pi G x}{3\delta^2}\left(\frac{8\pi G}{3}(1-x)Q\right)^{-(1+x)/(1-x)}(-\sin^2(2\delta P) + 2\sin^2(\delta P)\cos(2\delta P)) - \left(\frac{\mathrm{d}\kappa}{\mathrm{d}Q} - \frac{8\pi G}{3}\frac{\mathrm{d}(mg/\ell_0 a)}{\mathrm{d}Q}\right)\cos(2\delta P) + \frac{\mathrm{d}\log\eta}{\mathrm{d}Q}\left(\left(\frac{8\pi G}{3}(1-x)Q\right)^{-2x/(1-x)}\frac{1}{2\delta^2}(\sin^2(2\delta P) - 2\sin^2(\delta P)\cos(2\delta P)) + \kappa - \frac{8\pi G}{3}\frac{mg}{\ell_0 a(Q)}\right)\right). \tag{A4}$$

The same trigonometric identities as in (40) then imply that $\ddot{Q}$ depends linearly on $\cos(2\delta P)$, and our remaining results go through.

APPENDIX B: SADDLE-POINT ANALYSIS

The background on-shell action for the solution (36), here setting $\kappa_0 = 1$, has a strikingly similar form compared with the classical one,

$$S_0 = -\frac{3q_1^2}{4M} + \frac{1}{2}Mq_1(-3 + \delta^2(\Lambda - 3))\left(\frac{\Lambda}{3} - 1\right) + \frac{1}{324}M^3(\Lambda - 3)^2(\delta^2(\Lambda - 9) - 3)(\delta^2(\Lambda + 3) - 3). \tag{B1}$$

For saddle points, $\partial S_0/\partial M = 0$, we once again get four solutions. Their analytic forms are still somewhat involved,

$$M = -\frac{3\sqrt{q_1}}{\sqrt{(3-\Lambda)(\delta^2(\Lambda+3)-3)}}, \tag{B2}$$

$$M = \frac{3\sqrt{q_1}}{\sqrt{(3-\Lambda)(\delta^2(\Lambda+3)-3)}}, \tag{B3}$$

$$M = -\frac{3\sqrt{q_1}}{\sqrt{(3-\Lambda)(\delta^2(\Lambda-9)-3)}}, \tag{B4}$$

$$M = \frac{3\sqrt{q_1}}{\sqrt{(3-\Lambda)(\delta^2(\Lambda-9)-3)}}. \tag{B5}$$

On analyzing the conditions for their denominators to remain real, we find that

$$|\delta| < \frac{1}{\sqrt{\Lambda/3+1}} \quad \text{if } \Lambda > 3 \tag{B6}$$

or

$$|\delta| > \frac{1}{\sqrt{\Lambda/3+1}} \quad \text{if } \Lambda < 3 \tag{B7}$$

for the first two solutions, and

$$|\delta| < \frac{1}{\sqrt{\Lambda/3-3}} \quad \text{if } \Lambda > 9 \tag{B8}$$

or

$$|\delta| > \frac{1}{\sqrt{\Lambda/3-3}} \quad \text{if } 3 < \Lambda < 9 \tag{B9}$$

for the other two, while $\Lambda < 3$ does not imply real solutions in this case.

Thus, for sub-Planckian Λ, there are at least two imaginary solutions, and all four solutions are imaginary if $|\delta| < 1/\sqrt{2}$ [the limiting case for $\Lambda \to 3$ in (B7)].

For larger Λ, all four solutions may be real provided $|\delta| < 1/\sqrt{2}$.

Without holonomy modification, $\delta = 0$, there are only two saddle-point solutions, both either real or purely imaginary depending on the value of Λ. Interestingly, in none of these cases does the reality of the saddle points depend on the value of q_1, unlike in Einstein gravity. The reason for this is that we assume $\kappa/\ell_0^2 = q$ for the spatial curvature in our specific solution, which is a possible behavior of the inverse-triad term only near $q \sim 0$ (and assuming a specific power-law behavior). As we go to larger q, especially near $q = q_1$, $\kappa \approx 1$, as it should, and analytical solutions are more difficult to come by.

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