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Martin Bojowald and Suddhasattwa Brahma Phys. Rev. Lett. **121**, 201301 — Published 13 November 2018 DOI: 10.1103/PhysRevLett.121.201301

Loops rescue the no-boundary proposal

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New and non-trivial properties of off-shell instantons in loop quantum cosmology show that dynamical signature change naturally cures recently observed problems in the semiclassical path integral of quantum gravity. If left unsolved, these problems would doom any theory of smooth initial conditions of the universe. The no-boundary proposal, as a specific example of such a theory, is rescued by loops, presenting a rare instance of a fruitful confluence of different approaches to quantum cosmology.

A major ambition of quantum cosmology is to derive properties of the universe from a theory of quantum gravity combined with a specific selection of initial conditions at the big bang. There have been two main proposals of initial conditions, the no-boundary wave function [1] and the tunneling picture [2]. They have been unified recently, but also came under new scrutiny [3, 4] by an application of Picard–Lefschetz theory to the Lorentzian path-integral of quantum gravity. An extension to perturbative and non-perturbative deviations from spatially isotropic geometries has revealed two possible outcomes, each of which would eliminate the attraction of a theoretical proposal setting conditions at the very beginning of the universe: Either there are run-away perturbations [5–8], or, at the very least, the initial conditions have to be amended by hand so as to achieve stability, a latetime property [9]. The problem is very general and can be traced back to geometrical properties of space-time in general relativity. Only a modified space-time structure can overcome such an obstruction. As we will see, this happens rather naturally in loop quantum cosmology.

A different scenario has been developed for some time in loop quantum cosmology [10, 11]. Initially, in exactly homogeneous cosmological models there were several indications [12–14] that quantum space-time effects could lead to a bounce at large (Planckian) density, such that the expanding part of the universe may have been preceded by collapse. The inclusion of inhomogeneity in a covariant fashion, as perturbations [15, 16] or nonperturbatively within spherical symmetry [17–19], then revealed an unforeseen implication of the same spacetime effects that resolve the singularity: At large density, the universe has the structure of a certain 4-dimensional Euclidean geometry in which the usual time direction of Lorentzian space-time is replaced by a fourth spatial dimension [20, 21]. Crucially, this dynamical signature change, unlike classical versions, is non-singular [22].

Nothing can propagate if there is only space, and therefore the original bounce picture is altered. However, the emergence of Euclidean space is strikingly similar to the technical implementation of the no-boundary proposal, which posits that the classical form of expanding spacetime is "rounded off" by a Euclidean cap replacing the big-bang singularity. In this letter, we show that the analogy is not just a formal one: The main difficulties of the no-boundary proposal, found in [5, 6], can be resolved if the Lorentzian path integral is augmented by some of the quantum-geometry effects found in loop quantum cosmology. In particular, off-shell instantons in loop quantum cosmology are subject to signature change even if the energy density is significantly sub-Planckian.

The specific forms in which Euclidean space makes its appearance in the no-boundary proposal and in loop quantum cosmology, respectively, are quite different from each other. In the no-boundary proposal, the origin of Euclidean space is a combination of the formal Wick rotation often employed in quantum-field theory — replacing real time t with complex time $\tilde{t} = \pm it$ — with the selection of specific saddle points to evaluate a semiclassical path integral. As a consequence of Wick rotation, a standard cosmological line element becomes Euclidean in the new coordinate \tilde{t} , as in

$$ds^{2} = -N(t)^{2}dt^{2} + a(t)^{2}d\Omega_{k}^{2} = \tilde{N}(\tilde{t})^{2}d\tilde{t}^{2} + \tilde{a}(\tilde{t})^{2}d\Omega_{k}^{2} = 1$$

for an isotropic cosmological model with spatial line element $d\Omega_k^2$, k = 0 or $k = \pm 1$ indicating the curvature of space. The new scale factor, $\tilde{a}(\tilde{t})$, describes how constant- \tilde{t} hypersurfaces grow as \tilde{t} increases, but since \tilde{t} has lost its meaning as time, it no longer describes dynamical growth. The lapse function N(t) specifies the rate of progress of time t. The way it appears in (1) shows that a coordinate-independent Wick rotation can be formulated by replacing N with $\tilde{N} = \pm iN$, leaving t unchanged.

Loop quantization: Loop quantum cosmology does not introduce complex coordinates or complex lapse functions. Instead, it is based on quantum modifications of spatial or space-time geometry which in the broader setting of loop quantum gravity [23, 24] have been found to facilitate the technical implementation of a quantum theory of gravity in terms of a Hilbert space and well-defined operators. In particular, the basic continuum quantities of spatial geometry, such as areas and volumes, are represented by operators with discrete spectra [25–27]. Moreover, an infinitesimal change of these quantities in time — or, more geometrically, the extrinsic curvature of space in space-time — no longer has a linear and local expression in space but is instead exponentiated and extended one-dimensionally, along an eponymous loop [28, 29]. In a cosmological model such as (1), two new effects are implied [30]: (i) There is no operator that directly represents extrinsic curvature \dot{a} or the Hubble parameter \dot{a}/a , and (ii) an operator version of a^2 has a discrete spectrum.

Effect (i) leads to holonomy modifications of cosmological equations: While spatial non-locality is not visible in homogeneous cosmological models, the specific form of non-linearity realized in loops implies that there are operators only for periodic functions such as $\sin(\ell(a)\dot{a})/\ell(a)$ with a function (or constant) $\ell(a)$ depending on quantization ambiguities. Any polynomial appearance of \dot{a} , as in the Friedmann equation, should therefore be approximated by trigonometric holonomy functions before it can be loop quantized. If $\ell(a) \approx \ell_{\rm P}/a$ with the Planck length $\ell_{\rm P}$ (a choice made in [31]), the new version differs from the classical Friedmann equation only near Planckian curvature. There are noticeable on-shell effects only around the big bang, but there they may be significant.

A discrete spectrum as in effect (ii) leads to strong deviations from continuity only for quantities sensitive to the spacing, which for an area such as a^2 would be tiny (Planckian). However, another consequence is that an operator with a discrete spectrum containing the zero eigenvalue, as is the case for a^2 , does not have an inverse operator, usually defined by inverting the eigenvalues. The need to quantize $1/a^n$ for different choices of n, for instance to obtain well-defined matter Hamiltonians, can be fulfilled by using commutators [32] such as

$$\hat{h}^{-1}[\hat{h},\sqrt{\hat{a}}] = -\frac{1}{2}\hbar\ell a^{-1/2}$$
(2)

where $\hat{h} = \exp(i\ell\hat{p}_a)$, using the momentum $p_a \propto \dot{a}$, is a "holonomy" operator or a quantization of \dot{a} that exists in loop quantum cosmology. The left-hand side of (2) does not require the non-existing inverse of an operator with discrete spectrum containing zero, and yet an operator with an inverse power of a in the classical limit results on the right [33]. Using such commutator versions implies stronger deviations from the continuum than the spacing of the *a*-spectrum alone would indicate, in particular for small values of *a* which may be relevant near the big bang. An analysis of these new operators [34, 35] shows that the eigenvalues $(a^{-1})_i$ of well-defined inverse operators of a are related to the eigenvalues a_j of a by $(a^{-1})_j =$ $f(a_i)/a_i$ with a function $f(a_i)$ that approaches $f(a_i) =$ 1 for large a_j and, for small a_j , is approximated by a power-law form $f(a_i) \approx a_i^n$ with a positive integer n > 2. The small-a behavior eliminates the divergence of a direct

inverse at $a_j = 0$. The precise form of $f(a_j)$ and the small-*a* power *n* depends on quantization ambiguities.

Both loop effects result from geometrical considerations independent of common quantum effects such as fluctuations. In a first approximation, they can therefore be studied with a modified version of the Friedmann equation (or the corresponding Hamiltonian) in which any appearance of \dot{a} is written trigonometrically, and any inverse of a is replaced by an appropriate power of $a^{-1}f(a)$. In order to capture the main effects contained in the two functions $\ell(a)$ and f(a), we replace the classical Hamiltonian (constraint) underlying the Friedmann equation,

$$C_{\text{class}} = -\frac{3}{8\pi G}a\left(\frac{\dot{a}^2}{N^2} + k\right) + m(a) = 0$$
 (3)

using a generic matter energy m(a), with

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

Here, $Q = a^3/(4\pi G)$ and $P = -\dot{a}/(Na)$ are canonical variables. We have assumed a specific *a*-dependence of the first ambiguity function, $\ell(a) = \delta a^{-1}$, $\delta \sim \ell_{\rm P}$, motivated by previous studies that suggested a preference for this behavior; see, for instance, [16]. Our results can be generalized to a power-law behavior $\ell(a) \propto a^{2x}$, but independently indicate the same preference for x = -1/2.

Suitable powers of the inverse-*a* correction function f(a) lead to a function $\kappa(Q)$ in the curvature term $(\kappa(Q) = k$ classically), and to a factor g(Q) multiplying the matter energy m(Q). Following the canonical procedure, one then derives the modified Friedmann equation

$$\left(\frac{\dot{a}}{Na}\right)^2 = \left(\frac{8\pi G}{3}\frac{m(a)g(a)}{a^3} - \frac{\kappa(a)}{a^2}\right)$$
(5)
$$\times \left(1 + \delta^2 \frac{\kappa(a)}{a^2} - \frac{m(a)g(a)}{a^3\rho_{\rm QG}}\right)$$

with $\rho_{\rm QG} = 3/(8\pi G\delta^2)$.

Covariance: Any modification of general relativity must respect covariance in the sense that the degrees of freedom in the metric that correspond to coordinate choices do not contribute to observable quantities. The Friedmann equation of isotropic models tells us how the scale factor and matter change with respect to a time coordinate t that is compatible with the line element (1). Coordinate time t enters (3) or (5) only in the form Ndt, a term which is invariant with respect to coordinate changes $t \mapsto t'(t)$. Even after modifications by loop effects, such as the δ -term in (5), the isotropic model remains time reparameterization invariant. But the equation shows no information about covariance with respect to coordinate changes that mix space and time, such as $t \mapsto t'(t, x_i)$ where $x_i, j = 1, 2, 3$, are the spatial coordinates, because such transformations do not preserve

the form (1) of the line element from which (3) has been derived via Einstein's equation.

If one would like to test whether a modified Friedmann equation can be a part of a generally covariant theory, one should at least include perturbative inhomogeneity, such as the scalar and tensor modes prominent in early-unniverse cosmology, coupled to the scale factor of an isotropic background. In this setting, one can perform small coordinate changes of the form $t \mapsto t'(t, x_i)$ in addition to $x_i \mapsto x_i(t, x_j)$. Covariance under these transformations turns out to be highly restrictive. There are now four independent transformations, which must form a group or, in infinitesimal form, an algebra. If we consider a sufficiently small region such that spacetime is locally Minkowski, the classical transformations are given by the Poincaré algebra. Without perturbative inhomogeneity, by contrast, we only have the much simpler algebra given by time translations.

Modifying the Friedmann equation implies a modification of time translations. The issue of covariance, in a small, locally Minkowski region, is whether the modified time translation can be a part of a consistent (and perhaps modified) version of the Poincaré algebra. Canonical gravity provides methods to test this condition for a modification such as (4), which has been worked out in several models of loop quantum gravity.

The result is that covariant perturbations are possible, but they are such that the classical Poincaré algebra can no longer be used. In particular, at large curvature (large momentum δP) there is a crucial sign change in the commutator of a time translation with a boost. The same sign change is obtained if we use the classical Poincaré algebra but replace the time translation with a space translation, and the boost with a rotation. In this way, the modification in (4) or (5) for $\delta \neq 0$ implies signature change when δP is large. In some cases, it can be shown [36, 37] that the redefined line element

$$\mathrm{d}s_{\beta}^2 = -\beta N^2 \mathrm{d}t^2 + a(t)^2 \mathrm{d}\Omega_k \tag{6}$$

instead of (1) is consistent with the modified Poincaré relations where β is the function that determines the sign change in the time-boost commutator. When $\beta < 0$ at large curvature, signature change is explicit.

Signature change: Signature change as it appears in models of loop quantum gravity is, therefore, rather different from the version used in the no-boundary proposal. We will now show that it can have important consequences in the same context. In particular, as the main result, we can use a Lorentzian path integral — that is, an integral over paths weighted by $\exp(iS/\hbar)$ rather than $\exp(-S/\hbar)$ — and have stable perturbations. To do so, we need, as the major new ingredient, off-shell instantons which do not solve (5) but rather the secondorder equation of motion of the background theory. (Noboundary initial conditions are formulated with respect to gauge-fixed time, such that the first-order equation is no longer enforced. In this way, the Euclidean cap — a non-classical property — can be realized in a semiclassical path integral.) Such solutions then have to be extended by a covariant theory of perturbative inhomogeneity.

In order to facilitate a comparison with derivations in [6], we will assume that $8\pi Gm/a^3 = \Lambda$ is a cosmological constant, choose a lapse function N = M/a with constant M, write the modified Friedmann equation in terms of $q = a^2$, and derive a second-order equation for this variable. We will then solve the second-order equation, (7) below, without imposing the first-order one, (5), thus dealing with off-shell Lorentzian instantons, as is required to carry out the no-boundary path integral. Several unexpected cancellations will make sure that the function β in (6) remains meaningful for off-shell instantons. Moreover, and also surprisingly, such off-shell β do not require large densities to be negative. These new features are the reason why loop quantum cosmology is able to rescue the no-boundary proposal.

Deriving the second-order equation for q leads to

$$\ddot{q} = \frac{2}{3}\Lambda M^2 \left(1 - \frac{3}{\Lambda} \frac{\mathrm{d}\kappa}{\mathrm{d}q} + \delta^2 \left(1 - \frac{3}{\Lambda} \frac{\kappa}{q} \right) \left(2 \frac{\mathrm{d}\kappa}{\mathrm{d}q} - \frac{\kappa}{q} - \frac{\Lambda}{3} \right) \right)$$
(7)

The right-hand side of (7) is always regular in q thanks to inverse-a corrections; the no-boundary initial value q(0) = 0 can therefore be imposed. For small t, q and κ/q are small and the right-hand side of (7) is approximately constant. A generic small-t behavior of $q(t) \propto t + O(t^2)$, as in [6] but possibly with modified coefficients, then follows. A discussion of stability requires only the small-tbehavior.

Identifying small t with the early universe in models of loop quantum gravity, one could expect that signature change is automatically realized. However, this result is far from clear. Signature change has been derived for on-shell solutions which obey the first-order Friedmann equation. The second-order equation used for off-shell instantons has a larger solution space to which standard result do not necessarily apply. Moreover, signature change in models of loop quantum gravity requires strong quantum space-time effects, which are usually found only at large, near-Planckian curvature: The canonical analysis that ensures covariance implies that the function β to be used in (6) has the form $\beta(P) = \cos(2\delta P)$ [16, 17, 38]. It takes the value $\beta(P) = -1$ if $\delta P = \pi/2$, such that $\sin(\delta P) = 1$ and (4) implies Planckian matter density if $\delta \sim \ell_{\rm P}$. One of the advantages of the no-boundary proposal, however, is that it might be able to explain the origin of the universe without referring to uncertain Planckian effects — its initial stage merely assumes a small cosmological constant without any high-density matter or radiation. If loop quantum gravity could imply earlytime stability only at the expense of requiring Planckian physics, it would not be of much use in rescuing the noboundary proposal.

Fortunately, several new properties conspire to solve these two problems in one strike. In particular, it is possible to derive a consistent off-shell β as a function of the scale factor using only the second-order equation. (Technical details are provided in the supplementary material.)

Written as a function of q(t), this new β is given by

$$\beta(t) = \frac{1 - \delta^2 M^{-2} \left(\ddot{q} + \frac{1}{2} \dot{q}^2 / q \right)}{1 - \frac{2}{3} \delta^2 \Lambda} \,, \tag{8}$$

using small dg/dq and $d\kappa/dq$. For sub-Planckian Λ , the denominator is close to one. For small-t no-boundary solutions, we have $q(t) \approx ct$ with constant c > 0, and

$$\beta \approx 1 - \frac{\delta^2 c}{2M^2} \frac{1}{t} < 0 \tag{9}$$

is negative as long as $t < \frac{1}{2}\delta^2 c/M^2$. Rather surprisingly, but crucially, off-shell instantons in loop quantum cosmology imply signature change even for sub-Planckian energy densities or Λ . The advantage of the no-boundary proposal being independent of Planckian physics is therefore not destroyed by bringing in signature change from loop quantum gravity.

Timeless stability: We are now in a position to draw our main conclusions. The results of [5, 6] are based on a detailed analysis of the Lorentzian path integral, paying special attention to suitable contours when integrating over the lapse function. The path integral is Lorentzian in that one integrates over real N, eliminating the Wick rotation to imaginary $\tilde{N} = \pm iN$ in (1) suggested by the original Hartle–Hawking proposal. Picard–Lefschetz theory is then used to improve the convergence property of this highly oscillatory integral, shifting the integration contour for N into the complex plane (but not all the way to the imaginary axis).

Since we are interested here in stability properties, we do not need an explicit calculation of a path integral. However, we make use of a crucial property observed and explained in [6]: There are unbounded modes v of the metric which contribute to the path integral by an undamped Gaussian exponential $\exp(\lambda v^2)$ with the "wrong," positive sign of the exponent, $\lambda > 0$. Interpreting the path integral as a transition amplitude, instability is implied because metric perturbations v are not suppressed. But how is it possible that the Lorentzian path integral, integrating the bounded $\exp(iS/\hbar)$ for real lapse functions, results in real undamped Gaussians for some modes? Picard-Lefschetz theory deforms the integration contour such that certain complex N are used in integrations, but it does not change the value of the original real integral if there are no poles in the complex plane.

A crucial insight of [6] explains this puzzle by noting that the integrand has a branch cut on the real M-axis. The contour must bypass this branch cut by deviating slightly into the upper imaginary half-plane, and in this way picks up complex actions from complex M. (The contour must be above the branch cut to access the relevant saddle point which lies in the first quadrant of M.)

Undamped Gaussians in the Lorenztian path integral are a direct consequence of this branch cut. Specifically, [6] use the equation $\ddot{v} \approx -\frac{1}{4}c^{-2}M^2\ell(\ell+2)v/t^2$ for a spherical harmonic tensor mode v of moment ℓ , using a no-boundary background q(t) = ct. This equation is solved by $v_{\pm}(t) = v_1 t^{\frac{1}{2}(1\pm\gamma)}$ (with $v_1 = v_{\pm}(1)$) where $\gamma = \sqrt{1 - \ell(\ell+2)M^2/c^2}$ clearly shows the branch cut on the M-axis. Moreover, the action evaluated on the regular solution v_+ is equal to $S_+(v_1) = \frac{1}{4}M^{-1}(\gamma - 1)v_1^2$ and has a negative imaginary part above the branch cut. Inserting the imaginary S_+ in $\exp(iS/\hbar)$ leads to an undamped Gaussian in the path integral of perturbations. Our strategy is now to show that signature change from loop quantum cosmology moves the branch cut to the imaginary M-axis, such that the argument of [6] no longer applies: The integrated action is always real and does not lead to undamped Gaussians.

For small t, as shown in more detail in the supplementary material, derivations of consistent perturbation equations in models of loop quantum gravity [16] imply that we have the mode equation

$$\ddot{v} \approx \frac{1}{4} \left((n-2\epsilon)(n+2) + \epsilon(\epsilon+2) - \beta \frac{M^2 \ell(\ell+2)}{c^2} \right) \frac{v}{t^2}$$
(10)

with $\epsilon = -1$ for our β while $\epsilon = 0$ (and n = 0) classically. We still have solutions $v_{\pm} = v_1 t^{\frac{1}{2}(1 \pm \gamma)}$, but now

$$\gamma = \sqrt{1 + n(n+2) - \beta \frac{\ell(\ell+2)M^2}{c^2}}.$$
 (11)

With dynamical signature change in an intermediate range of t, that is $\beta < 0$, γ is always real for real M. Its branch cuts in the complex plane are now on the imaginary M-axis where they do not affect the Lorentzian path integral, while the qualitative structure of saddle points remains unchanged. The argument for Gaussians with positive exponents, given in [6], no longer applies, and indeed the action S_+ is always real and finite.

Most importantly, in the asymptotic regime of small t using (9), the dominant term in (10) is $\ddot{v} \approx \frac{1}{4}\alpha v/t^3$ with $\alpha = 2\delta^2 \ell(\ell+2)/c > 0$. This equation has a regular solution given by a modified Bessel function of the second kind, $v(t) = v_1 \sqrt{t} K_1(\sqrt{\alpha/t})/K_1(\sqrt{\alpha})$. The action,

$$S(v_1) = \frac{\sqrt{\alpha}}{4M} \frac{K_0(\sqrt{\alpha})}{K_1(\sqrt{\alpha})} v_1^2, \qquad (12)$$

is again real and finite and no undamped Gaussians result. Signature change is crucial here because these properties would be different if $\alpha < 0$, as is the case for $\beta > 0$.

Our new combination of the Lorentzian path integral with results from loop quantum cosmology is surprisingly productive. Loop quantum cosmology has led to an unexpected new property of quantum space-time by suggesting non-singular, dynamical signature change in the early universe. This effect strengthens the original intuition behind the no-boundary proposal by replacing the technical notion of Euclidean path integrals with dynamical signature change embodied by an effective line element (6). Moreover, it is just what the no-boundary proposal, or any theory of a smooth beginning, needs in order to imply stable perturbations without imposing final conditions. While these are quantum-gravity effects, they do not require a Planckian energy density or cosmological constant.

Acknowledgements: The authors are grateful to Job Feldbrugge, Jean-Luc Lehners, and Neil Turok for discussions, and to the Perimeter Institute for Theoretical Physics for hospitality. Research at Perimeter Institute is supported by the Government of Canada through Innovation, Science and Economic Development, Canada and by the Province of Ontario through the Ministry of Research, Innovation and Science. This work was supported in part by NSF grant PHY-1607414. S.B. is supported in part by the Ministry of Science, ICT & Future Planning, Gyeongsangbuk-do and Pohang City and the National Research Foundation of Korea grant no. 2018R1D1A1B07049126.

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