Landscape of polymer quantum cosmology

Lautaro Amadei, Alejandro Perez, and Salvatore Ribisi
Aix Marseille University, Université de Toulon, CNRS, CPT, 13007 Marseille, France

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We show that the quantization ambiguities of loop quantum cosmology, when considered in wider generality, can be used to produce discretionary dynamical behavior. There is an infinite dimensional space of ambiguities which parallels the infinite list of higher curvature corrections in perturbative quantum gravity. There is, however, an ensemble of qualitative consequences which are generic in the sense that they are independent of these ambiguities. Among these, one has well-defined fundamental dynamics across the big bang, as well as extra microscopic quantum degrees of freedom that might be relevant in discussions about unitarity in quantum gravity. We show that, in addition to the well-known bouncing solutions of the effective equations, there are other generic types of solutions for sufficiently soft initial conditions in the matter sector (tunneling solutions) where the scale factor goes through zero and the spacetime orientation is inverted. We also show that, generically, a contracting semiclassical universe branches off at the big bang into a quantum superposition of universes with different quantum numbers. Despite their lack of quantitative predictive power, these models offer a fertile playground for the discussion of qualitative and conceptual issues in quantum gravity.

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I. INTRODUCTION

Quantum field theories with local degrees of freedom generically suffer from divergences due to uncontrolled UV contributions to amplitudes. At the mathematical level the latter can be traced to the fact that interactions involve products of fields (operator valued distributions in quantum field theory) at the same spacetime point and that such products are ill defined if constructed naively. The standard procedure of renormalization eliminates infinities from the physical amplitudes at the price of introducing counterterms with free parameters to be fixed by a series of renormalization conditions taken from physical inputs. In certain simple situations one can instead take due care in the definition of products of operator valued distributions and thus completely avoid, from the very beginning, UV divergences (see for instance [1]). However, such a procedure is not unique, and free parameters also arise in the regularization procedure. These parameters must be fixed (in order to produce physical amplitudes) by the same number of renormalization conditions of standard textbook treatments. In this way there is a formal link between the number of counterterms necessary to eliminate UV divergences and regularization ambiguities.

A key difficulty of canonical approaches to quantum gravity is that such intrinsic ambiguity of standard quantization recipes appears to be out of control. This is associated with the nonrenormalizability of the gravitational interaction, which in the case of general relativity in metric variables, is illustrated by the fact that the family of general covariant functionals of g_{ab} representing a possible action principle describing the quantum effective action is infinite dimensional and that the parameter controlling the dimensionality of such free couplings is the quantum gravity coupling itself. In other words,

$$S[g_{ab}] = \frac{1}{2\kappa}\int \sqrt{|g|}(R + \Lambda + \alpha_1 \ell_p^2 R^2 + \alpha_2 \ell_p^4 R^3 + \cdots + \beta_1 \ell_p^2 R_{\mu\nu\alpha\sigma} R^{\mu\nu\alpha\sigma} \cdots) dx^4, \tag{1.1}$$

where only some representative terms have been written with dimensionless couplings $\alpha_1, \alpha_2, \cdots, \beta_1, \beta_2, \cdots$, etc. Generic radiative corrections produce divergences that need to be cured by counterterms in correspondence with the infinite number of elements in the previous general action, requiring infinitely many renormalization conditions and compromising the predictive power of the approach.[1] However, from the previous formal discussion, an equivalent concern threatens nonperturbative formulations where UV divergences are avoided via clever choices of variables and/or mathematical structures, as the problem of divergences metamorphoses into the appearance of ambiguities.

As a complementary remark one must keep in mind that the previous analysis sometimes strongly depends on the "fundamental variables" chosen for quantization. An example of this is the emblematic case of gravity in three

[1] It is possible, however, that these couplings would flow under the renormalization group in a nontrivial way toward some asymptotic fixed point characterized by a finite amount of parameters. Such a perspective, known as the asymptotic safety scenario [2], is the subject of active investigations [3].

dimensions where a naive metric variable analysis would lead to similar conclusions as in four dimensions. However, when the most general action is written in terms of first order variables, one discovers that there is only a finite dimensional set of possibilities. Namely,

$$S[e,\omega] = \frac{1}{2\kappa}\int e_I \wedge F_{IJ}(\omega)\epsilon^{IJK} + \Lambda e_I \wedge e_J \wedge e_K \epsilon^{IJK} + \alpha S_{\rm CS}(\omega), \tag{1.2}$$

where e^I_a is a triad field, ω^{IJ}_a is a Lorentz connection, and $S_{\rm CS}(\omega)$ is the Chern-Simons action. The theory is indeed integrable; it has only global or topological degrees of freedom, and its quantization is free of (infinite dimensional) ambiguities [4,5]. Strikingly, a similar finite dimensionality of the space of gravity actions is valid in first order variables in four dimensions, where one has that the most general gravitational action is given by

$$S[e^A_a,\omega^{AB}_a] = \frac{1}{2\kappa}\int \overbrace{\epsilon_{IJKL}e^I\wedge e^J \wedge F^{KL}(\omega)}^{\text{Einstein}} + \overbrace{\Lambda\epsilon_{IJKL}e^I\wedge e^J\wedge e^K\wedge e^L}^{\text{Cosmological Constant}} + \overbrace{\alpha_1 e_I\wedge e_J\wedge F^{IJ}(\omega)}^{\text{Holst}} + \underbrace{\alpha_2(d_\omega e^I\wedge d_\omega e_I - e_I\wedge e_J\wedge F^{IJ}(\omega))}_{\text{Nieh−Yan}} + \underbrace{\alpha_3\ell_p^2 F(\omega)_{IJ}\wedge F^{IJ}(\omega)}_{\text{Pontrjagin}} + \underbrace{\alpha_4\ell_p^2\epsilon_{IJKL}F(\omega)^{IJ}\wedge F^{KL}(\omega)}_{\text{Euler}}, \tag{1.3}$$

where $d_\omega e^I$ is the covariant exterior derivative of e^I and $\alpha_1\cdots\alpha_4$ are dimensionless coupling constants. For nondegenerate tetrads, Einstein's field equations follow from the previous action independently of the values of the α's: the additional terms are called topological invariants, describing global properties of the field configurations in spacetime. The α_1 term is called the Holst term [6], the α_2 term is the Nieh-Yan invariant, the α_3 term is the Pontryagin invariant, and the α_4 term is the Euler invariant. Despite not changing the equation of motion, these terms can actually be interpreted as producing canonical transformations in the phase space of gravity.[2]

The previous facts motivate the idea of the pertinence of such variables for the implementation of nonperturbative quantization and thus can be viewed as the natural rationale behind the approach of loop quantum gravity [12] (although the history of the subject cannot be reduced to such a perspective but rather to the discovery of Ashtekar's new variables [13]). However, not surprisingly, unlike the simple 3D case (which has no local degrees of freedom) the absence of ambiguities in quantum theory remains an open question. Indeed, at early stages of the development of loop quantum gravity, it was found that—thanks to the peculiar Hilbert space of quantum gravity adapted to diffeomorphism invariance and the Ashtekar-Barbero connection variables—the quantum gravitational dynamical equations (embodied by the Hamiltonian constraint that encodes both the gravity and matter interactions) were free of UV divergences [14]. Nevertheless, the quantization of the Hamiltonian constraint suffers from ambiguities of an infinite dimensional nature, suggesting that the renormalizability issue is still present [15].

However, there is an unresolved consistency check concerning the quantization of the constraints in loop quantum gravity. This is the issue of anomalies. More precisely, the quantum dynamical equations are represented by a set of quantum operators that must satisfy a commutation algebra inherited from the classical algebra of generators of the surface deformation algebra. Checking the absence of anomalies has shown to be a remarkably difficult task, suggesting that such a consistency check could reduce the ambiguities in the definition of the quantum constraints [16–18]. However, one should recognize that such a result is not clear from the general perspective of our initial discussion, as the algebra of surface deformations is a feature of any diffeomorphism invariant formulation of gravity. More precisely, in the case of metric variables, the canonical analysis of the general action (1.3) would produce the same surface deformation algebra independently of the values of the undetermined couplings.

The nontriviality of this question has motivated recent interest in the application of renormalization group methods to investigate (as in asymptotic safety scenarios) the possibility that the nonperturbative techniques of loop quantum gravity could help uncover a nontrivial UV completion of the theory [19–24].

The perspective that we emphasize here is not new [15], but its full implications in quantum cosmology have been somewhat underestimated. The problem of quantization ambiguities in the cosmological models inspired by the full theory has been considered in various works [25]; however, under certain restrictive assumptions that reduce the discussion to finite dimensional sectors of the space of ambiguities [26–30], it has been argued not to represent a threat to the predictability of the framework. Our present

[2]In such a context, the so-called Immirzi parameter [7] corresponds to the combination $\gamma \equiv \frac{1}{(\alpha_1+2\alpha_2)}$ [8]. This parameter plays a central role in the spectrum of quantum geometric operators, and controls, in the presence of fermions, the strength of an emergent four-fermion interaction [9–11].

analysis shows that, as long as the question of ambiguities remains open in the full theory, polymerized symmetry reduced models cannot produce accurate quantitative predictions but only qualitative insights. We show here that the ambiguities inherited from the full theory have an important dynamical effect on these models that, naturally, compromises their predictive power. Nevertheless, due to their simplicity, our analysis does not reduce, in any way, the great value of these models for illustrating qualitative features of quantum gravity. Some of these features are, in simple models at least, generic (i.e., independent of the ambiguity issue), suggesting that they might represent robust features possibly realized in nature.

The paper is organized as follows. In Sec. II we reproduce the FLRW dynamical equations, and its corresponding Hamiltonian version, in unimodular gravity. The formalism is completely equivalent to general relativity but offers the advantage of resolving the so-called problem of time in quantum gravity: instead of a Hamiltonian constraint there is a nonvanishing Hamiltonian evolving in unimodular time. This is an advantage that simplifies the analysis in quantum theory. In particular, we show that (when the matter sector is represented by a massless scalar field) the dynamical equations are equivalent to those of a nonrelativistic particle scattering in a potential well represented by the matter Hamiltonian. Such an analogy simplifies the discussion of the impact of the regularization ambiguities in the Hamiltonian, addressed in Sec. III. It should be clear, however, that conclusions we draw are expected to hold in the other formulations where instead of a Hamiltonian one has to deal with a Hamiltonian constraint (but where the quantum dynamics remains difficult to compute and most approaches simply deal with effective evolution equations). In Sec. III we focus on two infinite dimensional families of regularization ambiguities: in Sec. III A we introduce the notion of holonomy corrections, while in Sec. III B we discuss inverse volume corrections. Other ambiguities exist—like factor ordering ambiguities or other ambiguities stemming from the details of the translation of the quantization scheme proposed in the full theory down to cosmology (e.g., μ_0 vs. $\bar{\mu}$ regularization, etc.). However, the ones we discuss are the most representative infinite dimensional families and thus the ones that most clearly compromise the predictability of these models. In Sec. IV we investigate the influence of the ambiguities in the quantum dynamics. Remarkably, many aspects of quantum theory are computable in the unimodular framework. This is again due to the simple translation of the cosmological problem to the scattering of a nonrelativistic particle in a potential. In Sec. V we show that it is possible to write the effective dynamical equations for an arbitrary polymer regularization (the technical results that lead to such equations are presented in Appendix). In Sec. VI we investigate the solutions of the effective equations for a general polymerization function and exhibit the most salient properties in terms of generic features of the regularizing function. The freedom in the polymerization function can be tuned to obtain discretional dynamical evolution. We present a few examples of this in Sec. VI D, where, for instance, inflation (without an inflaton) is induced by holonomy corrections. Concluding remarks are given in Sec. VII.

II. UNIMODULAR QUANTUM COSMOLOGY AS A SIMPLE TESTING GROUND

In order to show the influence of the regularization ambiguities on physical quantities, one first needs to be able to perform explicit calculations within the framework where these ambiguities appear. Even when quantum cosmology models correspond to classical systems with finitely many degrees of freedom, the nonstandard representation theory used in the construction of quantum theory makes these models sufficiently complicated (in some versions) to prevent explicit calculations. For example, different choices of time variables (realized by different choices of lapse functions) produce different quantum constraints, which can present supplementary challenges when it comes to analyzing the quantum dynamics.

This is, in part, the reason why the technique of the so-called effective dynamics has been developed [31], where the quantum evolution is approximated by modified classical equations of motion. These effective equations are affected by the ambiguities in the definition of the quantum dynamics. In fact, these modifications are supposed to encode the quantum corrections to general relativity coming from quantum gravity. In this sense the quantization ambiguities on which we focus here are expected to affect these quantum corrections. However, explicitly showing the form of the effective equations can be challenging or (unnecessarily) more involved when different time variables are chosen. In order to simplify our presentation, we analyze cosmology in the unimodular version of general relativity. Unimodular gravity is simply equivalent to standard general relativity if the matter coupling is diffeomorphism invariant [32]. When applied to cosmology, it has the advantage of resolving the problem of time as the lapse function is fixed by the unimodular constraint. In the literature of quantum cosmology, it is customary to modify the scalar constraint by assuming different choices of the lapse function (a choice that it is often referred to as a “gauge choice”). Even when unimodular gravity is not a gauge fixing of standard general relativity, from the previous perspective unimodular cosmology could be characterized at the technical level by a choice of lapse. We see that such a choice makes the Hamiltonian evolution particularly simple in the gravity sector and thus allows for the most transparent and simple derivation and resolution of the quantum as well as the effective dynamical equations. It should be clear that the main point of this work will not change if one uses a different notion of lapse. The choice we make has a very natural geometric interpretation that we describe in the following paragraph.

There is no preferred notion of time in general relativity. This implies that the dynamics is dictated by constraint equations and leads to the so-called problem of time in quantum gravity: instead of Schrödinger-like evolution equations, one has a timeless dynamics defined by the quantum constraints. This very complicated technical and conceptual problem can be circumvented in quantum cosmology by the use of tools that have become customary. The commonly accepted prescription is the use of some (partial) observable as a clock that allows for the deparametrization of the dynamics that leads to a Schrödinger-like evolution equation and the definition of the so-called physical Hilbert space of quantum cosmology. Even when such a procedure is not unique and thus might lead to unitarily inequivalent theories, this additional source of potential ambiguity does not concern us here. The reason why the problem of time is not as serious in quantum cosmology is the fact that, for the study of dynamical questions (sufficiently far form the Planckian regime), an effective classical description is available. Such a classical description allows us to deal with the problem of time in the usual way that is familiar to us in cosmology: via gauge fixing, i.e., particular choices with some clear interpretation ranging from comoving time, harmonic time, conformal time, and (our choice here) unimodular time.

Unimodular time is the time variable that naturally emerges from the description of cosmology in unimodular gravity [33]. Instead of a gauge fixing, unimodular gravity can be thought of as a genuine modified theory of gravity that is (apart from a subtlety in the cosmological constant sector) completely equivalent to general relativity. We use unimodular quantum cosmology [34,35] in what follows because, in this formulation, the gravitational part of the Hamiltonian takes a particularly simple form; indeed, the geometry degrees of freedom can be mapped uniquely to those of a nonrelativistic free particle. This feature allows for a very intuitive interpretation of both the effective classical evolution equations and the quantum gravity equations. In most situations of interest, the problem of quantum or classical evolution of geometry coupled with simple forms of matter can be seen as a regular scattering problem of a nonrelativistic particle in an external potential. This makes the setting of the dynamical system particularly appealing for its simplicity; however, it should be clear from our treatment that the implications drawn are of general validity and should apply (qualitatively speaking) to any of the customary parametrizations of loop quantum cosmology (LQC).

When specializing to (spatially flat) homogeneous and isotropic cosmologies with the metric

$$ds^2 = -N^2 dt^2 + a(t)^2 d\vec{x}^2, \tag{2.1}$$

the Einstein-Hilbert action supplemented with the unimodular constraint becomes

$$S = -\kappa^{-1} \int \left(\sqrt{|g|}R + \lambda(\sqrt{|g|} - 1) \right) dx^4 \tag{2.2}$$

where $\kappa = 16\pi G$, and λ is a Lagrange multiplier imposing the unimodular constraint $\sqrt{|g|} - 1 = 0$; we have put an overall minus sign in front of the action for later convenience. Specializing to the FLRW metric (2.1) one gets

$$S = \kappa^{-1} V_0 \int \left(6 \frac{a\dot{a}^2}{N} - \lambda(N|a|^3 - 1) \right) dt, \tag{2.3}$$

where total derivative terms have been eliminated, and the 3-volume V_0 of a fiducial cell has been introduced. Resolving the unimodular constraint fixes $N = |a|^{-3}$ and defines a preferred notion of time; from now on, we denote this new time variable as s and call it unimodular time. The action becomes

$$S = \kappa^{-1} V_0 \int 6a^4 \dot{a}^2 ds. \tag{2.4}$$

For further reference it is important to relate unimodular time with the standard comoving time τ, namely,

$$ds = -|a|^3 d\tau. \tag{2.5}$$

At this point we change variables to more convenient ones that make the action similar to that of a nonrelativistic free particle. The new configuration variable is given by the 3-volume density

$$x = a^3, \tag{2.6}$$

from which it follows that $\dot{x} = 3a^2\dot{a}$, and the action is then

$$\boxed{S = \int \frac{1}{2} m \dot{x}^2 ds}, \tag{2.7}$$

with

$$m \equiv \frac{4V_0}{3\kappa}, \tag{2.8}$$

where the dot denotes the derivative with respect to the unimodular time s. Note that the minus sign in front of (2.3) was chosen so that the kinetic term of the particle analog has the usual sign. Additionally, if we use the comoving time $d\tau = -ds/|a|^3$, we have

$$p = m\left(\frac{dx}{ds}\right) = -3m \frac{1}{|a|} \frac{da}{d\tau} = -3m \ \mathrm{sign}(a) H. \tag{2.9}$$

We see that the momentum variable in our parametrization is proportional to the Hubble rate H in the usual comoving variables. Let us introduce a scalar field as a matter model. Then, the matter action (with the same overall minus sign convention that we adopt) is

$$\begin{aligned} S_M &= \frac{1}{2}\int \sqrt{|g|}(\nabla_a\phi\nabla^a\phi + U(\phi))d^4x \\ &= -\frac{1}{2}V_0\int Na^3\left(\frac{1}{N^2}\left(\frac{d\phi}{ds}\right)^2 - U(\phi)\right)ds \\ &= -\frac{1}{2}V_0\int \left(a^6\left(\frac{d\phi}{ds}\right)^2 - U(\phi)\right)ds. \end{aligned} \tag{2.10}$$

Therefore, the action including our simple matter model is

$$S(x,\phi) = \int \left(\frac{1}{2}m\left(\frac{dx}{ds}\right)^2 - \frac{1}{2}V_0x^2\left(\frac{d\phi}{ds}\right)^2 - V_0U(\phi)\right)ds. \tag{2.11}$$

The previous action can be written in Hamiltonian form as

$$\boxed{S(x,\phi) = \int p\frac{dx}{ds} + p_\phi\frac{d\phi}{ds} - \left(\frac{p^2}{2m} - \frac{p_\phi^2}{2V_0x^2} - V_0U(\phi)\right)ds}, \tag{2.12}$$

where

$$p_\phi = -V_0x^2\frac{d\phi}{ds}. \tag{2.13}$$

A. Changing variables to match the standard setup

The previous (x, p) variables in the gravity sector were chosen to emphasize the simple link between unimodular gravity in the FLRW context and the dynamics of a point particle. A simple rescaling of these variables leads to the standard parametrization of the phase space in loop quantum cosmology in the so-called $\bar{\mu}$ scheme. The variables customarily used are (b, v), defined as

$$b \equiv -\frac{\gamma}{3m}p = -\frac{\gamma}{3}\frac{dx}{ds} = -\gamma a^2\frac{da}{ds} \tag{2.14}$$

and

$$v \equiv \frac{3m}{\gamma}x = \frac{V_0a^3}{4\pi G\gamma}. \tag{2.15}$$

Thus, one has

$$\{b, v\} = 1. \tag{2.16}$$

With these variables, the Hamiltonian is

$$H = \frac{V_0}{2\pi G\gamma^2}\left(\frac{3}{4}b^2 - \frac{p_\phi^2}{16\pi Gv^2} - 2\pi G\gamma^2U(\phi)\right), \tag{2.17}$$

which is proportional to the scalar constraint C as written in Ref. [36] [Eq. (2.19)] simply rescaled by the use of the unimodular time lapse, namely, $H = V_0C/(\pi G|v|)$. The advantage of using unimodular variables resides in the remarkable fact that the gravity part of the Hamiltonian depends only on the variable b (like a free particle in classical mechanics). This simple fact simplifies several technical as well as conceptual discussions of the classical and quantum features of the model.

III. REGULARIZATION AMBIGUITIES OF THE HAMILTONIAN

There are two aspects of the Hamiltonian that call for a modification of its classical expression in order to promote it to a well-defined self-adjoint operator in the special Hilbert space of loop quantum cosmology. One of them is that only quasiperiodic functions of b but not b itself can be quantized. The second is that inverse volume contributions to the Hamiltonian (entering through the matter coupling) are also modified by means of the use of classical expressions that eliminate their unboundedness at small volumes. Both modifications are ambiguous by nature and lead to dynamical effects that we analyze in what follows. Interest in this issue from the observational perspective has resurfaced recently in [37]; here we concentrate on further theoretical implications. There are other approaches for the definition of the quantum dynamics for cosmology where one starts from a more fundamental perspective at the quantum level and infers from it the symmetry reduced model [38–40]; we note that similar ambiguities are present in these perspectives as well. For simplicity, we concentrate on the loop quantum cosmology formulation where the problem is embodied in the notion of regularization.

A. Holonomy corrections

Due to the peculiar choice of representation in the quantization of the model (inspired by the structure of loop quantum gravity), there is no b operator in the Hilbert space of loop quantum cosmology but only operators corresponding to finite v translations [36,41], from here on referred to as shift operators,

$$\exp(i\lambda b) \rhd \Psi(v) = \Psi(v - \lambda), \tag{3.1}$$

where λ is some arbitrary length scale. As the classical Hamiltonian explicitly depends on b, it needs regularization in order to be promoted to a self-adjoint operator in the Hilbert space of loop quantum cosmology. Consequently, we replace (2.17) by

$$H = \frac{V_0}{2\pi G\gamma^2}\left(\frac{3f(\lambda b)^2}{4\lambda^2} - \frac{p_\phi^2}{16\pi G v^2} - 2\pi G\gamma^2 U(\phi)\right), \quad (3.2)$$

where

$$f(\lambda b) = \sum_{n\in\mathbb{Z}} f_n e^{in\lambda b}. \quad (3.3)$$

To be explicit about the regularization choice, we write the substitution rule as

$$\boxed{b^2 \to \frac{f(\lambda b)^2}{\lambda^2}}. \quad (3.4)$$

This operation is called polymerization in the loop quantum cosmology literature. Consistency with the classical dynamics imposes the following conditions: on the one hand, that $f(x) = \bar{f}(x)$, which translates into the condition

$$f_n = \bar{f}_{-n}. \quad (3.5)$$

On the other hand, one needs that

$$\langle f(\lambda b)\rangle = \lambda b_0 + \mathcal{O}[(\lambda b_0)^2] \quad (3.6)$$

for $\lambda b_0 \ll 1$ when expectation values are computed in suitable semiclassical states peaked at the classical momentum b_0. This second condition is necessary to recover the semiclassical dynamics of standard cosmology at low Hubble rates or the low density regime, leaving an infinite dimensional freedom in the choice of the regularized Hamiltonian to be promoted to an operator in the Hilbert space of our system. The standard choice in the loop quantum cosmology literature is $f_n = i\delta_n^1/2$, namely,

$$b^2 \to \frac{\sin^2(\lambda b)}{\lambda^2}. \quad (3.7)$$

A possible justification for this choice is that of simplicity. The link between such a choice in relation to the lowest nonvanishing eigenstate of the area operator in loop quantum gravity, and the special status given to the fundamental representation of the gauge group, is sometimes given as a further reason to use (3.7) (see [36]). This argument connects the regularization of a certain quantum operator in loop quantum cosmology to the features of a particular state (the state with minimal area eigenvalue) in loop quantum gravity. Even when accepting such a possibility, it is unclear how the lowest area eigenstate should play such a central role. Indeed, in quantum theory the principle of superposition rather suggests that states would typically be made of arbitrary superpositions of different area eigenvalues. Consideration of such aspects in full generality brings us back to the infinite dimensional landscape of polymerizations in (3.4).

When expressed in terms of the v basis, the evolution equation (related to the Hamiltonian constraint) contains a finite difference term, which, with the so-called traditional choice (3.7), becomes a discrete version of a second derivative in v. For an arbitrary choice (3.4) the finite difference term can be put in correspondence with a linear combination of the discretization of higher derivative terms in v. If one were looking for eigenstates of the Hamiltonian (3.2), one would be confronted with a growing multiplicity of formal solutions of the eigenvalue equation as the order of the corresponding difference equation grows when considering general functions $f(b)$ with arbitrarily high Fourier components. This question can be studied in the simpler context of the pure gravity case, which, in analogy with the point particle system, corresponds to the asymptotic, large universe regime, where standard matter contributions can be neglected using logic analogous to that of scattering theory. In such a simpler setting, most of these extra solutions related to the higher order character of the difference equation for arbitrary $f(b)$ are not normalizable and hence not part of the spectrum.

In the Wheeler-DeWitt standard representation of quantum cosmology, eigenstates of the Hamiltonian are doubly degenerate in correspondence with the two possible equal "energy" classical solutions corresponding to an expanding and/or contracting universe for a given cosmological constant: the two are related to the discrete symmetry $\dot{x} \to -\dot{x}$ involving the initial conditions of the theory written in the variables (2.11). Therefore, any additional degeneracy of energy eigenvalues would have no classical correspondence, and its associated conserved quantity would reveal the existence of new (microscopic) degrees of freedom. We postpone this discussion until Sec. IV.

The formal similarities with higher curvature corrections of the Einstein-Hilbert action due to quantum effects is manifest even when a rigorous statement is made difficult by the breaking of explicit covariance by the Hamiltonian formulation (in the first place) and by the further (possibly explicit) breaking of covariance introduced by the polymerization itself (see [42]). In perturbative quantum gravity, higher derivative terms arise from higher curvature corrections, and this changes the number of degrees of freedom as seen from a classical perspective. As higher curvature (higher derivative) terms appear multiplied by increasing powers of ℓ_p^2, all these corrections are taken to be negligible at energy scales well below the Planck scale. We believe that this analogy is interesting, thus making polymer models a nice simplified arena where difficult questions related to renormalization and the definition of the continuum limit can be explored in the highly simplified context of a model that (at least classically) starts with a finite number of degrees of freedom.

Finally, it is possible to exhibit the direct relation between the function $f(\lambda b)$ and the cosmological constant as follows. Standard considerations in unimodular gravity imply that [43,44]

$$\Lambda = 8\pi G \frac{E}{V_0}, \tag{3.8}$$

where E is the eigenvalue of (2.17) or (3.2). The discussion is simplified if we assume that we are in the massless scalar field case $U(\phi) = 0$. If a nontrivial self-interaction is present, then a more careful analysis is needed. We restrict ourselves to initial conditions given at $v = \pm\infty$ (large universes) where the contribution of the scalar field to the Hamiltonian (3.2) vanishes. In this limit the system is the analog of a nonrelativistic free particle where eigenvalues of the energy can be labeled by eigenvalues of momenta.[3] Therefore, from (3.2) one obtains the relation

$$\Lambda = \frac{3f^2(b_\infty)}{\gamma^2\lambda^2}, \tag{3.9}$$

where b_∞ is the asymptotic value of b for $v = \pm\infty$.

B. Inverse volume corrections

Inverse volume terms in the Hamiltonian introduce potential singularities in quantum theory. Such potential divergencies are present as well in the full theory of loop quantum gravity and need regularization when constructing a well-defined quantum scalar constraint operator. Thiemann introduced [45] a natural regularization of such potential UV divergences by realizing that inverse volume terms can be obtained from the Poisson algebra between well-defined geometric operators and the holonomy of the connection. In the case of cosmology the idea can be illustrated, for example, by the following simple classical identity,[4]

$$\frac{1}{\sqrt{|v|}} = \frac{2i}{\lambda}\,\mathrm{sgn}(v)\exp(i\lambda b)\{\exp(-i\lambda b), \sqrt{|v|}\}, \tag{3.10}$$

which suggests a natural regularization of quantities depending on the inverse volume using "holonomies" and commutators in the quantum theory. We use a symmetrized factor ordering, for instance,

$$\widehat{\frac{1}{\sqrt{|v|}}} \to \frac{1}{\hbar\lambda}\mathrm{sgn}(v)\Big(\exp(i\lambda b)[\exp(-i\lambda b), \widehat{\sqrt{|v|}}] + [\exp(-i\lambda b), \widehat{\sqrt{|v|}}]\exp(i\lambda b)\Big). \tag{3.11}$$

This choice regularizes the singular behavior of the inverse volume at $v = 0$—where the previous expression vanishes by construction—and produces a well-defined operator in the Hilbert space of loop quantum cosmology. However, the choice is by no means unique. In fact [in addition to factor ordering and other sources of ambiguities, such as the choice of the power of v inside the Poisson brackets in (3.10)] one has an infinite dimensional space of regularizations that is similar in spirit to the one identified for the regularization of curvature in (3.2) given by

$$\widehat{\frac{1}{\sqrt{|v|}}} \to \frac{\mathrm{sgn}(v)}{2\hbar\sum_{m\in\mathbb{Z}} c_m}\sum_{n\in\mathbb{Z}}\frac{c_n}{\lambda n}\Big(\exp(i\lambda nb)[\exp(-i\lambda nb), \widehat{\sqrt{|v|}}] + [\exp(-i\lambda nb), \widehat{\sqrt{|v|}}]\exp(i\lambda nb)\Big), \tag{3.12}$$

for arbitrary coefficients c_n. This implies that in addition to the infinite dimensional family of curvature regularizations, one has an (at least) equally large family of inverse volume regularizations, which would generically enter in the construction of the matter coupling when defining the quantum Hamiltonian. One can show that the action of the previous operator is simply given by (see [36])

$$\widehat{\frac{1}{\sqrt{|v|}}}\Psi(v) = \frac{\Psi(v)}{\hbar\sum_{m\in\mathbb{Z}} c_m}\sum_{n\in\mathbb{Z}}\frac{c_n}{\lambda n}\left(\sqrt{|v+\lambda n|} - \sqrt{|v-\lambda n|}\right) \equiv \frac{\Psi(v)}{\sum_{m\in\mathbb{Z}} c_m}\sum_{n\in\mathbb{Z}} c_n\left[\frac{1}{\sqrt{|v|}}\right]_n, \tag{3.13}$$

where we have introduced the definition

$$\left[\frac{1}{\sqrt{|v|}}\right]_n \equiv \frac{1}{\hbar\lambda n}\left(\sqrt{|v+\lambda n|} - \sqrt{|v-\lambda n|}\right). \tag{3.14}$$

One obtains

$$\sqrt{|v|}\left[\frac{1}{\sqrt{|v|}}\right]_n = 1 + \frac{1}{16}\frac{n^2\lambda^2}{v^2} + \frac{7}{128}\frac{n^4\lambda^4}{v^4} + \mathscr{O}\left(\frac{n^6\lambda^6}{v^6}\right), \tag{3.15}$$

which shows that, for a sufficiently large volume, one recovers the classical expected limit. Notice that the regularization (3.13) vanishes at $v = 0$. One can use the previous series expansion and choose the coefficients c_n in order to improve the convergence to the classical value. For example, with the choice

$$\begin{aligned} &\mathrm{c1} \to 9.42267, && \mathrm{c2} \to -13.1273,\\ &\mathrm{c3} \to 6.31659, && \mathrm{c4} \to -1.93791,\\ &\mathrm{c5} \to 0.355751, && \mathrm{c6} \to -0.0297957 \end{aligned} \tag{3.16}$$

one gets the regularization to coincide with $1/\sqrt{|v|}$ up to order $\mathscr{O}(n^{10}\lambda^{10}/v^{10})$ (plotted in blue in Fig. 1). One can

[3] More precisely, in our context these correspond to the eigenvalues of the shift operators (4.2), yet the key point is that they are still labeled by a value of b.

[4] This is a particular case of a more general identity leading to additional ambiguities [46]. For simplicity, we concentrate on the one given in [36].

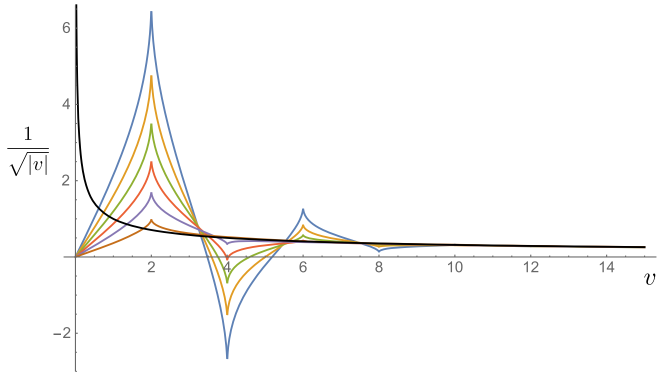

FIG. 1. Inverse volume corrections of the classical function $1/\sqrt{|v|}$ (shown in black). The blue curve represents the best approximation for large volumes, which coincides with the classical expression up to order $(\lambda/v)^{10}$. However, as the approximations get better for larger volumes, they get worse at Planckian volumes, as the plotted sequence illustrates, with deviations becoming the largest at low integer values times λ.

continue improving the convergence by eliminating higher order deviations from $1/\sqrt{v}$; it simply boils down to solving a linear system of equations with increasing dimension. One might think that such a process would produce a sequence of c_n converging pointwise to the Wilson-Ewing regularization [46,47] of the inverse volume, which is given by $1/\sqrt{|v|}$ for all $v \neq 0$, while it vanishes at $v = 0$. By plotting a few members of the above approximating sequence, we see that this will not be the case. In fact, the previous sequence, while it gets increasingly better at approximating $1/\sqrt{v}$ for large v, it differs more and more from the function $1/\sqrt{v}$ at around $v = \pm\lambda$ (see Fig. 1).

There are two important features that we would like to emphasize here. The first one is that the regularization of the inverse volume operator would lead to a function of v that is not differentiable everywhere due to the presence of the absolute value in the formulas. This is, of course, not a problem from the perspective of quantum theory where (for the quantum dynamics) only the evaluation of the regularization on a discrete lattice plays a role. However, at the nondifferentiable points the effective equations can simply not be trusted. The second important feature is that the regularization is a continuous function and thus bounded. We insist on the point that (even when some choices might seem natural given some subjective criteria) there is no well-defined rule that would actually eliminate the vast set of possibilities here either. We discuss some further consequences of inverse volume corrections later; in particular, in Sec. VI C, we see their role in the violation of the null energy condition near the big bang.

IV. QUANTUM THEORY: EVOLUTION ACROSS THE SINGULARITY

Let us discuss the main features of the quantum dynamics before discussing the validity of the effective dynamical approach that we use later for further interpretation—where the quantum dynamics is approximated by looking at the evolution of semiclassical states. One great advantage of the unimodular gravity formulation is that (at least in the FLRW context) the theory has a well-identified time evolution [in unimodular time (2.5)], and the kinematical Hilbert space of loop quantum cosmology is the physical Hilbert space. In other words, the problem of time is trivialized, and the physical interpretation of quantum theory becomes closer to that of standard quantum mechanics.[5] However, an important difference with standard quantum mechanics is the use of an unconventional representation of the basic phase space variables, which brings to the system a central property of the full theory of loop quantum gravity: fundamental discreteness. Concretely, instead of the standard Schrödinger representation on a gravitational Hilbert space of square integrable wave functions where v acts by multiplication and $b = -i\partial_v$, one introduces a Hilbert space where only the exponentiated version of b, the shift (or holonomy) operators $\exp i\lambda b$ (for arbitrary $\lambda \in \mathbb{R}$), are well defined. This is sometimes called the polymer representation, and the procedure of using this exotic representation (well motivated from the full theory) is called polymerization.

Consequently, there is no operator corresponding to b in the loop quantum cosmology polymer representation but only the operators corresponding to finite v translations [41], from here on referred to as shift operators defined as

$$\exp(i\lambda b) \rhd \Psi(v) = \Psi(v - \lambda). \tag{4.1}$$

States diagonalizing the shift operators are denoted $|b_0; \Gamma_\lambda^\epsilon\rangle$ and labeled by a real value b_0, where Γ_λ^ϵ is a 1D lattice of points, a graph, in the real line of the form $v = n\lambda + \epsilon$ with $\epsilon \in [0, \lambda)$ and $n \in \mathbb{N}$. The corresponding wave function of these eigenstates is given by $\Psi_{b_0}(v) \equiv \langle v | b_0; \Gamma_\lambda^\epsilon\rangle = \exp(-ib_0 v)\delta_{\Gamma_\lambda^\epsilon}$, where the symbol $\delta_{\Gamma_\lambda^\epsilon}$ evaluates to one when $v \in \Gamma_\lambda^\epsilon$ and vanishes otherwise. Assuming that $k = m\lambda$, it follows from (4.1) that

$$\exp(ikb) \rhd |b_0; \Gamma_\lambda^\epsilon\rangle = \exp(ikb_0)|b_0; \Gamma_\lambda^\epsilon\rangle. \tag{4.2}$$

The states $|b; \Gamma_\lambda^\epsilon\rangle$ are eigenstates of the shift operators which preserve the lattice Γ_λ^ϵ. The fact that these states are supported on discrete lattices (polymerlike excitations) is what motivated the name of the representation. Notice that the eigenvalues are independent of the parameter ϵ; i.e.,

[5] Closer but not exactly the same. Here, we are making reference to the uncomfortable questions related to the meaning of a quantum theory of the universe as a whole. These questions are indeed very important and remain open to a large extent. In order to concentrate on the main point of this paper, we have to ignore them altogether.

they are infinitely degenerate and span a nonseparable subspace of the quantum cosmology Hilbert space $\mathscr{H}_{lqc}$.

As the operator b does not exist in the Hilbert space, one has to construct approximations in terms of combinations of shift operators which behave like b in a suitable sense. This procedure is (as discussed in Sec. III A) intrinsically ambiguous. We would like to understand the influence of deviating from the standard regularization (3.7) to quantum dynamics. In order to do this we concentrate on the pure gravity case first. Indeed, the ambiguity (3.4) only affects the gravitational part of the Hamiltonian, and thus this simple case completely characterizes the dynamical influence of the choice of different regularization functions $f(\lambda b)$ in the quantum dynamics in the large volume asymptotic regime where matter dilutes until becoming negligible. Thus, we deal with the special case where, before quantization, the classical Hamiltonian is regularized as

$$H = \frac{b^2}{2m} \to \frac{f(\lambda b)^2}{2m\lambda^2}. \tag{4.3}$$

Note that this case is nontrivial because it admits a nonzero cosmological constant that is given by the value of the energy in the unimodular framework [recall (3.8)]. In quantum theory, we are interested in the eigenstates of the Hamiltonian (the analog of the time-independent Schrödinger equation). Let us first analyze the spectrum of the Hamiltonian in the traditional polymerization; namely, we would like to solve the equation

$$\left(\frac{\sin(\lambda b)^2}{2m\lambda^2} - E\right)|\Psi_E\rangle = 0, \tag{4.4}$$

which in the v basis becomes [due to (4.1)] the difference equation

$$\Psi_E(v-2\lambda) + \Psi_E(v+2\lambda) + (8m\lambda^2 E - 2)\Psi_E(v) = 0, \tag{4.5}$$

where the order of the difference equation is directly related to the polymerization choice. This seems to raise a potential difficulty: if instead of the traditional choice we take an arbitrary $f(\lambda b)$, the order of the difference equation will grow arbitrarily. Would this lead to an uncontrollable proliferation of spurious solutions? We will see that this is not the case. For the moment we continue the analysis of the present scenario. As the Hamiltonian is a combination of shift operators (4.1) of the kind for which one knows the eigenstates, one can simply express the energy eigenstates in terms of $|b_0;\Gamma^{\epsilon}_{2\lambda}\rangle$ (the eigenstates of the shift operators) and calculate the relationship between b_0 and the energy eigenvalues. We call these the polymerized dispersion relations. For the standard choice, energy eigenstates and dispersion relations are

$$|\Psi_{E(b_0)}\rangle = |b_0;\Gamma^{\epsilon}_{2\lambda}\rangle, \qquad E(b_0) = \frac{\sin(\lambda b_0)^2}{2m\lambda^2}. \tag{4.6}$$

A. The ϵ sectors

The previous energy eigenstates (eigenstates of the cosmological constant) are infinitely degenerate due to the ϵ degeneracy of the shift operators (4.1). This overabundance of solutions of the Schrödinger equation is controlled, in standard treatments, by fixing the volume lattice and choosing one ϵ sector. This choice is dynamically consistent because the Hamiltonian preserves the given lattice; however, in the presence of matter, the choice represents an additional dynamical ambiguity as the dynamical features depend on ϵ. This is particularly clear when we look at the inverse volume corrections of Sec. III B. Each different choice of ϵ gives a lattice that probes the volume regularization at different discrete points. As the inverse volume regularization enters the coupling of gravity with matter [see, for instance, Eq. (3.2)], the details of the dynamics will depend on this choice. Because the Hamiltonian preserves ϵ sectors, they are sometimes called superselection sectors. However, as there are other (Dirac) observables that do not preserve the lattice, these sectors are not superselected in any usual sense.

More precisely, in the case of pure gravity, observables commuting with the Hamiltonian and mapping between different values of ϵ (graph-changing observables) are simply the shift operators introduced in Sec. (4.1). In the case of a nontrivial matter coupling, other Dirac observables exist; they are technically hard to characterize explicitly in their full generality because of the usual difficulty associated with the construction of such conserved quantities. However, notice that if the matter coupling is such that matter dilutes as $v \to \infty$ (as expected for regular matter degrees of freedom), then shift operators remain Dirac asymptotic observables where the universe becomes large and the Hamiltonian tends to the pure geometry Hamiltonian in the usual sense of scattering theory. In this manner, the shift observables (4.1) define a complete set of commuting observables fully characterizing the positive energy (positive cosmological constant[6]) states. These asymptotic observables are like those regularly employed in standard situations involving scattering theory. Their existence shows that ϵ sectors are not superselected.

Hence, there is no clear reason to restrict to a single lattice, and superpositions of different lattices can be considered. Some of the implications of this possibility have been investigated in [43,44], where it is shown that these additional degrees of freedom, which are microscopic

[6]Negative Λ solutions exist in the presence of matter, and they correspond to bound states (in the analogous nonrelativistic particle system). These solutions do not reach the $|v| \to \infty$ asymptotic region and admit no scattering theory interpretation (as in the usual cases).

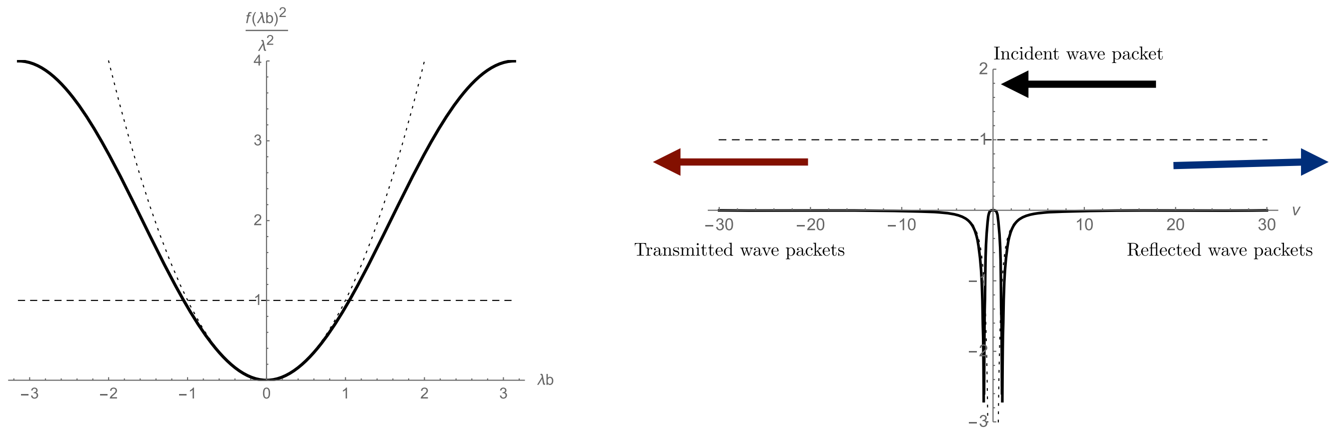

FIG. 2. Polymerization $f(x)^2 = -2(\cos(x) - 1)$ matching the degeneracy of eigenstates of the Schrödinger representation. On the right panel we show the different scattering channels in a matter coupling with a massless scalar that produces (for a given p_ϕ eigenstate) an effective potential regularized by inverse volume corrections (shown in black). The universe bounces into a superposition of transmitted and reflected modes with the same asymptotic (large v) Hubble rates. If we factor by the symmetry $v \to -v$, then we only have a bounce and the superposition disappears. The results of an analytically solvable model are shown in (4.10).

or Planckian, can be key in understanding the fate of information in situations where evolution across would-be singularities is relevant, like in cosmology and (most importantly) in the context of black hole formation and evaporation. In order to simplify the following discussion, we restrict our analysis to the case of states supported by a single lattice.

B. Degeneracy of the energy (cosmological constant) eigenstates in the pure gravity case

In the Schrödinger representation the dispersion relation is the familiar nonrelativistic particle relation $E(b_0) = b_0^2/(2m)$, which is doubly degenerate, corresponding to the momentum eigenstates with $b = \pm b_0$. Translating this to unimodular cosmology, these two eigenstates would correspond to a de Sitter state with a cosmological constant $\Lambda = 8\pi G E(b_0)/V_0$ that is either contracting or expanding in the FLRW slicing. With the standard polymerization (3.7), we first observe that a new degeneracy appears, as there are four different shift-operator eigenstates that produce the same energy, namely, those labeled by the four roots of the equation on the right of (4.6) depicted on the left of Fig. 2. We study the role of these additional solutions below after we describe this type of degeneracy for an arbitrary regularization.

For an arbitrary polymerization (3.4) the situation is quite similar. Eigenstates are again given by

$$|\Psi_{E(b_0)}\rangle = |b_0; \Gamma^\epsilon_{2\lambda}\rangle \quad \text{with} \quad E(b_0) = \frac{f(\lambda b_0)^2}{2m\lambda^2}. \tag{4.7}$$

However, the degeneracy of the energy eigenvalues is now dependent on the choice of the function $f(\lambda b)$. An example with six different eigenstates is depicted on the right panel of Fig. 4. In this example, one can distinguish two different situations. In the first case, the energy is E_1, and the eight solutions correspond to eigenstates of the form (4.7). In the other case, for the energy E_2, the number of solutions for the eigenvalue equation seen as a difference equation remains eight; however, only the four values of b_0 explicitly seen in the figure correspond to "plane-wave" eigenstates of the form (4.2). It is easy to show[7] that the other four solutions of the difference equation are diverging in either the $v \to \pm\infty$ limit and thus are not part of the Hilbert space (this is the analog of non-normalizable solutions of, for example, the time-independent Schrödinger equation for the harmonic oscillator). These additional solutions are most interesting when matter couplings that break v-translational invariance of the Hamiltonian are included.

C. Dynamical consequences when matter couplings are included

Here we show how the inclusion of matter couplings has the generic effect of producing "diffusion" in the various energy eigensectors, which would not be present in the Schrödinger quantization. The additional energy eigenvalues of the pure gravity model introduced by the choice of polymerization play an important dynamical role. We see that a universe starting in the large volume limit in one asymptotically de Sitter state—with a given cosmological constant (energy) and a given Hubble rate b_0—will "scatter" through the big bang into a superposition of the various eigenstates of the same asymptotic energy. In this way, the quantum dynamics of the bounce is much more complicated than hinted at by the effective equation approach, which will be discussed later. This is a simple instance of the physical expectation embodied in the statement that "anything that can happen happens in

[7] See, for instance, Sec. 2.3 of [48].

quantum mechanics." In a background-independent approach, the most likely result is that an initially semiclassical state (with a clear spacetime interpretation) will evolve into a superposition that might not always admit a single spacetime representation. Forgetting this simple fact about quantum mechanics is one of the current errors in setting up important questions such as the ones concerning the fate of information in black hole evaporation. Here, we again see how the present models of quantum cosmology represent a rich and valuable testing ground for conceptual ideas in spite of their limited quantitative predictive power, as far as observable effects are concerned.

One of the simplest models of matter coupling is that of a massless scalar field [i.e., $U(\phi) = 0$ in Eq. (2.10)]. In that case the momentum of the scalar field is conserved, and the gravitational dynamics is equivalent to that of a point particle (with kinetic energy $\propto b^2$) moving in an "external attractive potential" that goes as $\propto 1/v^2$ [see Eq. (2.17)]. The divergence in the potential is regularized in loop quantum cosmology using the Thiemann construction, which modifies the inverse volume dependence near the big bang at $v = 0$. Such a modification is illustrated in Figs. 2–4. Such a model is already complicated enough to make analytic calculations.

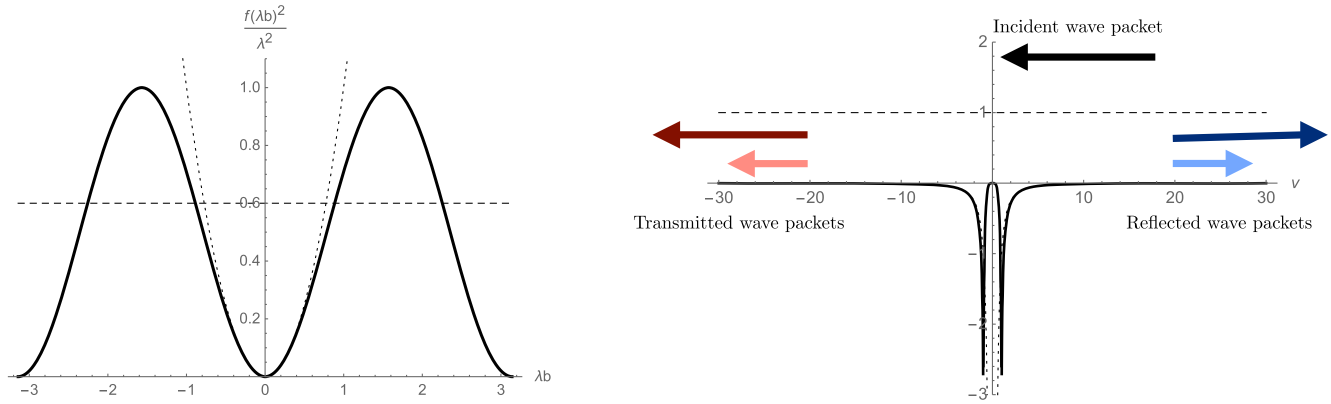

FIG. 3. New solutions in the traditional polymerization $f^2(x) = (\sin(x))^2$ (dispersion relations on the left). On the right panel we show the different scattering channels in a matter coupling with a massless scalar that produces (for a given p_ϕ eigenstate) an effective potential regularized by inverse volume corrections (shown in black). The universe bounces and tunnels in new channels with different asymptotic Hubble rates for a given cosmological constant. If the $v \to -v$ symmetry is imposed (as is customary in the specialized literature) the degeneracy remains, and the universe only bounces into the quantum superposition of two semiclassical solutions. The results of an analytically solvable model are shown in (4.10).

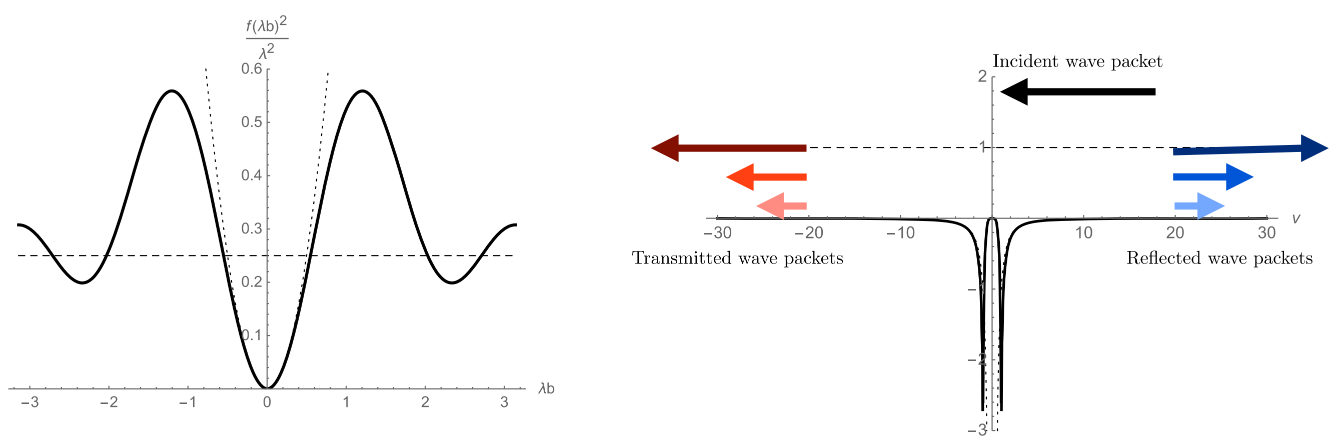

FIG. 4. Generic polymerization, where $f(x)^2 = 2/13(2 - (\cos[2x] + \cos[3x]))$. On the right panel we show the different scattering channels in a matter coupling with a massless scalar that produces (for a given p_ϕ eigenstate) an effective potential regularized by inverse volume corrections (shown in black). New channels for the bounce appear and a given universe evolves through the singularity into a quantum superposition of universes with the same cosmological constant (or expectation value of the cosmological constant for wave packets) but different Hubble rates. The results of an analytically solvable model are shown in (4.10).

However, the qualitative behavior that we illustrate does not depend on the details of the potential and only on the fact that the coupling with matter breaks the conservation of the variable b. This is simply due to the fact that matter couplings break translational invariance in the v axes, producing a nontrivial dynamics of the Hubble rate (a quite obvious fact from the standard classical perspective based on the Friedmann equations where the Hubble rate remains constant in the FLRW slicing only in pure de Sitter spacetime). Thus, the phenomenon we want to emphasize can be illustrated in a much simpler model where analytic calculations are trivial. An example of such a model is one in which the regularized $1/v^2$ potential produced by the corresponding contribution to the Hamiltonian (3.2) of the massless scalar field is replaced by the sum of two Kronecker deltas at $v=0$ and $v=\lambda$, in some way mimicking the two choices in the regularized potential seen in the previous figures. Notice, however, that this example is not meant to approximate the massless scalar field case in any precise sense. We only use it because we can solve it explicitly and because it produces the phenomenology that will be common (at the qualitative level) to any matter coupling. The only essential feature here is the breaking of translational invariance in the v axes.

Concretely, we concentrate on the difference equation

$$\Psi_e(v-2\lambda)+\Psi_e(v+2\lambda)+(e-2)\Psi_e(v)-\alpha\delta\left(\frac{v}{\lambda},1\right)\Psi_e(v) -\alpha\delta\left(\frac{v}{\lambda},0\right)\Psi_e(v)=0, \tag{4.8}$$

where $e\equiv 8m\lambda^2E$ and the delta functions are Kronecker deltas on the lattice $v=\lambda n$ with $n\in\mathbb{Z}$, and α is a coupling constant. This is a simple scattering problem, which is resolved via the ansatz

$$\Psi_e(v)=\begin{cases} e^{-ib_1(e)v}+R_1(e)e^{ib_1(e)v}+R_2(e)e^{ib_2(e)v} & (v\geq 0)\\ T_1(e)e^{-ib_1(e)v}+T_2(e)e^{-ib_2(e)v} & (v\leq 0),\end{cases} \tag{4.9}$$

where $b_1(e)>b_2(e)>0$ are the two positive solutions of the dispersion relation—plotted in Fig. 3—for the given value of e. The previous, discrete Schrödinger equation boils down to four independent linear equations from which one determines the reflection and transmission amplitudes. They are given by

$$R_1(e)=\frac{\alpha\left(i\alpha\sqrt{-(e-1)e}+\alpha(1-e)-(1-e)\left(e-i\sqrt{-(e-1)e}\right)\right)}{(e-1)(\alpha^2+e)} \qquad R_2(e)=\frac{i\alpha^2\sqrt{e}}{\sqrt{1-e}(\alpha^2+e)}$$

$$T_1(e)=\frac{e}{\alpha^2+e}-\frac{i\alpha\sqrt{e}}{\sqrt{1-e}(\alpha^2+e)} \qquad T_2(e)=\frac{\alpha\left(1+\frac{i\sqrt{e}}{\sqrt{1-e}}\right)e}{\alpha^2+e}. \tag{4.10}$$

There are two interesting limits of the previous result that will be relevant for the discussion in Sec. VI B: the reflection amplitudes vanish in the limit $\alpha\to 0$ where the bounce is completely suppressed, while the transmission amplitudes vanish in the hard-scattering limit $\alpha\to\infty$. Here, we use a simplistic model where we can make explicit calculations. As mentioned before, the qualitative features present in this model remain in the realistic case (this is confirmed by numerical simulations, which we have omitted for simplicity).

The results shown in Figs. 2–4 can be understood in a simple, intuitive way as follows. The left panel of each of these figures shows the regularization of the "kinetic" energy part of the Hamiltonian (in the framework given in analogy to the nonrelativistic point particle). Instead of a quadratic dependence in b (shown by the dotted curve), the kinetic energy is represented by a more general periodic function depending on the regularization choice. This implies that, for a given total energy (see the horizontal dotted line on the left panels of the three figures), there is a multiplicity of possible classical solutions—more than the usual pair of solutions for the quadratic kinetic energy. In the scattering process, due to the interaction with the potential, a particular incident wave (corresponding to one with the wave numbers b whose kinetic energy matches the total energy) will scatter into a superposition of all the others. When the kinetic energy is quadratic, one gets the usual superposition of reflected and transmitted solutions. In the general regularization case more channels are opened and generically excited by any potential breaking translational invariance (so that b is no longer conserved). This qualitatively explains the results illustrated in the figures. Computing the actual amplitudes requires solving the quantum dynamical equations as we have done in our simplified model.

V. MODIFIED COSMOLOGICAL EFFECTIVE EQUATIONS

Let us start from the unimodular Hamiltonian constraint where (3.2) is equated to some energy value that plays the role of the cosmological constant, namely,

$$C \equiv \mathcal{H} - V_0 \frac{\Lambda}{8\pi G} = \frac{V_0}{2\pi G\gamma^2}\left(\frac{3f(\lambda b)^2}{4\lambda^2} - \frac{p_\phi^2}{16\pi G v^2} - 2\pi G\gamma^2 U(\phi) - \frac{1}{4}\gamma^2\Lambda\right) \approx 0. \tag{5.1}$$

We study the evolution of the volume variable

$$v = \frac{V_0 a^3}{4\pi G\gamma}, \tag{5.2}$$

$$\frac{d\langle v\rangle}{ds} = -i\langle[v,\mathcal{H}]\rangle \approx -\frac{\partial\langle\mathcal{H}\rangle}{\partial b} = -\frac{3V_0}{4\pi G\gamma^2\lambda} f'(\lambda b) f(\lambda b) \tag{5.3}$$

where we have used the results of Appendix in the derivation of the effective equations, the prime denotes derivatives with respect to λb, and s denotes unimodular time given in terms of comoving (cosmic) time τ by

$$ds = -|a|^3 d\tau = -\frac{4\pi G\gamma}{V_0}|v| d\tau. \tag{5.4}$$

Indeed, the previous equation gives us an expression for $\dot{a}/a$, namely,

$$\frac{\dot{a}}{a} = \frac{1}{\gamma\lambda} f'(\lambda b) f(\lambda b). \tag{5.5}$$

From now on, we denote $\langle v\rangle$ simply by v. Using the standard definition of the Hubble rate $H \equiv \dot{a}/a$, we can write

$$H^2 = \frac{1}{\gamma^2\lambda^2} f'(\lambda b)^2 f(\lambda b)^2. \tag{5.6}$$

The constraint (5.1) can be rewritten as

$$\boxed{C = \frac{3V_0}{8\pi G\gamma^2\lambda^2}\left(f(\lambda b)^2 - \frac{\rho_\phi + \rho_\Lambda}{\bar{\rho}}\right) \approx 0} \tag{5.7}$$

where $\rho_\Lambda \equiv \Lambda/(8\pi G)$, ρ_ϕ is the scalar field contribution to the energy density,

$$\bar{\rho} = \frac{3}{8\pi G\gamma^2\lambda^2}, \tag{5.8}$$

and

$$\rho = \rho_\phi + \rho_\Lambda = \frac{p_\phi^2}{32\pi^2 G^2\gamma^2 v^2} + U(\phi) + \frac{\Lambda}{8\pi G} = \frac{\dot{\phi}^2}{2} + U(\phi) + \frac{\Lambda}{8\pi G} \tag{5.9}$$

is the standard energy density. This implies

$$f(\lambda b) = \sqrt{(\rho/\bar{\rho})}. \tag{5.10}$$

It is also convenient to introduce the pressure

$$P = \frac{p_\phi^2}{32\pi^2 G^2\gamma^2 v^2} - U(\phi) - \frac{\Lambda}{8\pi G} = \frac{\dot{\phi}^2}{2} - U(\phi) - \frac{\Lambda}{8\pi G}. \tag{5.11}$$

Thus, we arrive at the modified Friedmann equation

$$\boxed{H^2 = \frac{8\pi G\rho}{3}\left[f'\left(f^{-1}\left(\sqrt{\rho/\bar{\rho}}\right)\right)\right]^2.} \tag{5.12}$$

We now look at the evolution equation of the energy density (5.9),

$$\frac{d\langle\rho\rangle}{ds} = -i\langle[\rho,\mathcal{H}]\rangle = -i\frac{3V_0}{8\pi G\gamma^2\lambda^2}\langle[\rho, f(\lambda b)^2]\rangle = \frac{3}{8\pi G\gamma^2\lambda^2}\frac{d\langle f(\lambda b)^2\rangle}{ds} \tag{5.13}$$

where the Hamiltonian is $\mathcal{H} = 3V_0 f(\lambda b)^2/(8\pi G\gamma^2\lambda^2) - V_0\rho$. Now, using Remark 4 from the Appendix we obtain

$$\frac{d\langle\rho\rangle}{ds} = \frac{3}{16\pi G\gamma^2\lambda^2}\frac{V_0\langle p_\phi^2\rangle}{(4\pi^2 G^2\gamma^2)v^3} 4\lambda f'(\lambda b) f(\lambda b) = \frac{3V_0\langle p_\phi^2\rangle}{16\pi^3 G^3\gamma^3 v^3} H. \tag{5.14}$$

An important corollary of the previous algebra (or simply from Remark 4) is that

$$\dot{b} = -4\pi G\gamma(\rho + P)\frac{|v|}{v}, \tag{5.15}$$

which follows directly from Remark 4, the definition of ρ and P; the sign comes from the relationship (5.4) between comoving time τ and unimodular time s. Now, using (5.4) we get the continuity equation

$$\boxed{\dot{\rho} + 3H(\rho + P) = 0} \tag{5.16}$$

where the quantities in the equation are expectation values. It is now a simple exercise to show that from (5.16) and (5.12), the *modified* Raychaudhuri equation is as follows:

$$\dot{H} = -4\pi G(\rho+P)\Big[f'\Big(f^{-1}\Big(\sqrt{\rho/\bar{\rho}}\Big)\Big)^2 + f''\Big(f^{-1}\Big(\sqrt{\rho/\bar{\rho}}\Big)\Big)f\Big(f^{-1}\Big(\sqrt{\rho/\bar{\rho}}\Big)\Big)\Big]. \quad (5.17)$$

This concludes the derivation of the effective cosmological equations for arbitrary regularizations of the Hamiltonian encoded in the arbitrary function $f(\lambda b)$. We see that in regions where the latter behaves linearly as in (3.6), one recovers the standard classical Einstein equations in the cosmological context. However, and this is the key point of our paper, deviations from the Einstein equations can be introduced by "tuning" the function $f(\lambda b)$. Such modifications, as we will see, have important physical consequences and thus make the large number of Fourier coefficients in $f(\lambda b)$ relevant ambiguity parameters, compromising the use of these models for physical predictions.

VI. LANDSCAPE OF POLYMERIZED MODELS OF QUANTUM COSMOLOGY

In this section we analyze the generic implications of the effective dynamical equations. We assume their validity through the region corresponding to the would-be singularity of classical cosmology where the scale factor a approaches zero. For certain, suitable, initial, semiclassical states for contracting universes, this approximation might hold true in some cases (for instance, for suitable bouncing solutions); however, we know from our analysis in Sec. IV that the state of the universe branches off into other solutions that go through the $a=0$ regime. In these other branches the effective dynamical equations break down unless one considers a rather artificial regularization of the inverse volume corrections. Thus, such solutions can only be understood in full generality using quantum theory. Due to this behavior we call these solutions tunneling solutions.

A. Bouncing branches

We first study the bouncing solutions of the effective equations, which are usually described in the LQC literature, analyzing the generic effect of the choice of polymerization function $f(\lambda b)$. We recall equation (5.5),

$$\frac{\dot{a}}{a} = \frac{1}{\lambda\gamma} f'(\lambda b) f(\lambda b), \quad (6.1)$$

where $f'(\lambda b)$ denotes the derivative with respect to λb. We also need the modified Raychaudhuri equation (5.17), which can be written in the form

$$3\frac{\ddot{a}}{a} = -4\pi G((\rho+3P)f'^2 + 3(\rho+P)f''f). \quad (6.2)$$

From (5.15) and assuming the validity of the null energy condition (NEC), $\rho + P \geq 0$, we can determine the direction of change of b depending on the sign of the volume of the universe. This greatly simplifies the analysis of the landscape dynamics. NEC are violated due to quantum gravity effects when inverse volume corrections in the matter coupling are taken into account. However, this is not relevant for the bouncing branches for states such that the effective equations are valid, as the bounce prevents v from reaching the regions where NEC are violated (see Sec. VI C).

Critical points in the function $f(\lambda b)$ correspond to two possibilities: bounces (minimum volume configurations where the universe stops contracting and starts expanding) and turning points (maximum volume configurations where the volume of the universe stops increasing and starts decreasing). Such situations are identified by the condition $\dot{a}=0$, which, from (6.1), arises when $f=0$ or $f'=0$. We first study the case $f'=0$. In order to understand if we are at the bounce or turning point, we have to study the sign of the second derivative of the volume (a bounce occurs for $\ddot{v}>0$, a turning point for $\ddot{v}<0$). Evaluating (6.2) at points where $f'=0$, we obtain

$$\frac{\ddot{a}}{a}\Big|_{f'=0} = -4\pi G(\rho+P)f''f. \quad (6.3)$$

Assuming that the NEC is valid, local maxima of the function f represent a bounce when $f>0$ as well as for local minima of f when $f<0$. Conversely, we have turning points at local minima of f for $f>0$ and at local maxima of f for $f<0$. What about the points where $f=0$? If the cosmological constant is positive, then the form of the Hamiltonian imposes that

$$f^2(\lambda b) \geq \sqrt{\frac{\rho_\Lambda}{\rho_c}}. \quad (6.4)$$

Thus, these points are inside a "classically forbidden" region, but they can be reached by setting $\Lambda = 0$. In this case they become a special case of points where $f(\lambda b)^2\rho_c = \rho_\Lambda$. In general, in de Sitter asymptotic configurations (Minkowski being a limiting case), the contributions of other forms of matter to ρ and P vanish. This is illustrated in Fig. 5. Assuming that the universe is in the $v>0$ branch, Eq. (5.15) implies that $\dot{b} \leq 0$ as long as the NEC holds with $\dot{b}=0$ in the de Sitter configurations where $\rho + P = 0$. These configurations are fixed points of the flow of b (recall that b is simply related to the Hubble rate according to the classical analysis from where we started).

With all this information, we can qualitatively interpret the situation described in Fig. 5 by observing that it represents two distinct possible histories for the universe. The first starts in the classically allowed region on the right in an (asymptotically) de Sitter state defined by the furthest intersection of $f(\lambda b)$ with $\sqrt{\rho_\Lambda/\rho_c}$ to the right. The universe

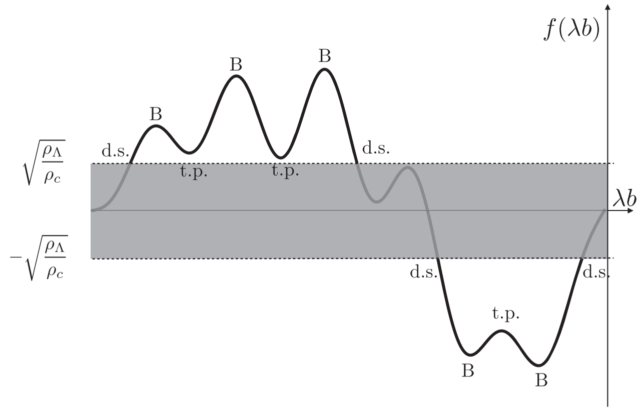

FIG. 5. Illustration of the dynamical features from a generic $f(\lambda b)$ when assuming $\Lambda \geq 0$. If we require $\rho \geq 0$, we have a bound on f given by $f^2 \geq \rho_\Lambda/\bar{\rho}$. Close to λb_0 with $f^2(\lambda b_0) = \rho_\Lambda/\bar{\rho}$, the function must be well approximated by $f(\lambda b) \approx \pm\lambda(b - b_0)$ in order to recover general relativity at low regular matter densities. We denote bounce points by B, turning points by t.p., and fixed points where the universe becomes asymptotically de Sitter by d.s. Note that the difference between the two branches [given by positive and negative values of $f(\lambda b)$] is only apparent as the constraint (5.7) depends on $f^2(\lambda b)$. The effective equations do not allow the universe to go from one branch to the other (however, in the quantum regime there could be tunneling as discussed in Sec. IV).

contracts and exits the purely de Sitter state, entering a phase where other forms of matter start to play a dynamical role. At the first minimum the universe bounces for the first time and starts expanding. The expansion continues until the universe reaches the first maximum (from right to left), where it starts contracting again until the second minimum is reached, and a last bounce leads to an expanding universe that expands forever towards a final asymptotic de Sitter state. A second sequence of events can be described in a similar fashion for the evolution along the classically allowed region on the left of Fig. 5.

Note that the initial and final asymptotic de Sitter phases are described by different Hubble rates, and the former are modulated by the value of f'^2 at the asymptotic points according to (5.12). One could introduce an effective cosmological constant at such de Sitter fixed points,

$$\Lambda_{\mathrm{ds-fp}} \equiv \Lambda f'^2. \tag{6.5}$$

Notice that these fixed points correspond to low energy regions where the density of matter (other than the cosmological constant) goes to zero. More generally, one can expand the modified Friedmann equation (5.12) around an arbitrary density ρ_0 and write

$$\frac{\dot{a}^2}{a^2} = \frac{8\pi G_{\mathrm{eff}}}{3}\rho + \frac{\Lambda_{\mathrm{eff}}}{3} + \mathcal{O}\left(\frac{(\rho - \rho_0)^2}{\rho_c^2}\right). \tag{6.6}$$

A simple calculation gives

$$G_{\mathrm{eff}} = G(f'^2 + f'' f) \tag{6.7}$$

and

$$\Lambda_{\mathrm{eff}} = (f'^2 + f'' f)\Lambda - 8\pi G\rho_0 f f''. \tag{6.8}$$

For $\rho_0 = \Lambda/(8\pi G)$ we recover the de Sitter fixed point value (6.5). Notice that as we approach a bouncing point, G_{eff} becomes negative, making gravity repulsive. The same functional dependence of G_{eff} is responsible for the effect interpreted as a change of signature in [49].

Finally, in the case of $\Lambda < 0$ there is a nontrivial lower bound for ρ given by $\rho_{\mathrm{min}} = -\rho_\Lambda$ corresponding to points where $f = 0$. In the point particle analogy these are turning points of a bound state where the kinetic energy vanishes; here, $f(\lambda b) = 0$. For the universe these are turning points where the universe achieves minimal regular matter density before recollapsing into a denser regime. The other qualitative features at critical points remain the same as in the previous discussion.

B. Tunneling branches (in the case of a massless scalar field)

In Sec. IV, we have shown that the quantum theory predicts that, in addition to the traditional bounce evoked in the previous discussion and advocated in the LQC literature, the universe can also tunnel across the singularity into an expanding phase. The bounce is clearly captured by the effective equations. Can tunneling also become apparent from these equations? It is possible to see this if one considers inverse volume corrections in the matter coupling described in Sec. III B. It is possible to see this if one considers inverse volume corrections in the matter coupling which are nontrivial for macroscopic universes. However, for generic inverse volume corrections whose effects happen in the UV, no semiclassical description is available and the phenomenon of tunneling can only be understood quantum mechanically.

For simplicity, we concentrate on the case of a massless scalar field. Assuming that we are in an eigenstate of the momentum π_ϕ (conserved in this case), we have already observed that its contribution to the Hamiltonian (3.2) can be seen as an effective potential in analogy to a nonrelativistic particle parametrization of Sec. II. However, this contribution is now finite everywhere, as the $1/v^2$ classical behavior is regularized by the Thiemann trick. This means that there must exist solutions of the effective equations where the universe evolves through $v = 0$ (or the scale factor $a = 0$) into $v < 0$ without experiencing the bounce produced by the kinetic term when the variable b reaches the suitable critical points of $f(\lambda b)$ described above. For this to happen the universe must scatter through the big bang singularity "softly" in the sense that the variable b

must not reach one of the critical points of $f(\lambda b)$. This occurs when the universe—interpreted as the point particle—rolls down the potential

$$V(v) \equiv -p_\phi^2 \left[\frac{1}{v^2}\right]_{\text{reg}} \tag{6.9}$$

in such a way that its "kinetic energy" does not grow beyond the bound

$$\begin{aligned} \frac{p_\phi^2}{4\pi G\gamma^2} \max \left[\frac{1}{v^2}\right]_{\text{reg}} &\leq \frac{3}{\gamma^2\lambda^2} f^2(\lambda b_c) - \Lambda \\ &= \frac{3}{\gamma^2\lambda^2}(f^2(\lambda b_c) - f^2(\lambda b_\infty)). \end{aligned} \tag{6.10}$$

We observe that, as the regularized potential is bounded, for $|p_\phi|$ sufficiently low the universe experiences (according to the effective equations) a soft transition from $v > 0$ to $v < 0$ in finite unimodular time Δs instead of a bounce. The scale factor crosses $a = 0$; however, there is no singularity as one can easily check from the effective equations (6.1) and (6.2) and the fact that both P and ρ vanish there. Indeed, the universe goes through a de Sitter phase where Λ dominates. Even when $a = 0$ is reached in finite unimodular time s, the would-be singularity $a = 0$ is reached at infinite comoving time τ. If valid, the effective equations predict an infinite number of e-folds of inflation around the soft transmission from $v > 0$ to $v < 0$. Even when there is only one such transition, in spirit the scenario resembles the eon transition of conformal cyclic cosmology proposed by Penrose [50]. However, these conclusions are not accurate for inverse volume regularizations that modify the matter coupling from the expected classical behavior around the Planck scale only.

Concretely, if we take the standard inverse volume correction based on $[1/\sqrt{v}]_1$ [recall Eq. (3.14)], we obtain

$$\max \left[\frac{1}{v^2}\right]_{\text{reg}} = \frac{4}{\lambda^2\hbar}, \tag{6.11}$$

$$p_\phi^2 \leq 3\pi\ell_p^2(f^2(\lambda b_c) - f^2(\lambda b_\infty)). \tag{6.12}$$

However, we see that in order for the previous conclusions to hold, the effective equations would have to be valid in the description of the universe from $v = \lambda$ to $v = -\lambda$. If λ is of the order of the Planck scale, then it is clear that the details of the dynamics evoked above (de Sitter inflation for an unlimited number of e-folds) do not survive in the fundamental description where the variable v jumps to discrete values of the order of λ. However, the conclusion that the transmission channel exists, in addition to the well-known bouncing channel, remains. A precise analysis of such transitions would require using a fully quantum treatment, which is of course possible.

In this respect it is interesting to revisit the results of Sec. IV in light of the present discussion. Notice that, qualitatively speaking, the parameter α regulating the strength of the toy-model potential in (4.10) is the analog of p_ϕ^2 here. Even when nonvanishing, the transmission amplitudes go to zero in the limit $\alpha \to \infty$, and only the bouncing channels remain. Consideration of the quantum theory uncovers a feature that we evoked previously. Indeed, the criterion for soft bounce (6.10) loses its quantitative relevance, and we realize that even if one considers unbounded regularizations such as the one proposed in [46,47], there will be a wave function component in the transmission sector in addition to the bouncing sector for suitable initial states that probe the potential on sufficiently soft points of the potential. More precisely, consider the regularization where

$$\left[\frac{1}{v^2}\right]_{\text{reg}} = \frac{1}{v^2} \quad \forall\, v \neq 0, \quad \text{while} \left[\frac{1}{0^2}\right]_{\text{reg}} = 0. \tag{6.13}$$

We study a semiclassical state defined on a lattice of $v = n\lambda$ with $n \in \mathbb{Z}$, i.e., a superposition of volume eigenstates that will evolve on this lattice in such a way that the potential will be probed only on such lattice points. In this case the criterion (6.10) can be written as

$$p_\phi^2 \leq p_{\rm C}^2 \equiv 12\pi\ell_p^2(f^2(\lambda b_c) - f^2(\lambda b_\infty)), \tag{6.14}$$

which cannot be a sharp bound because its construction relies on the effective dynamics. However, it remains an order-of-magnitude criterion in the sense that as p_ϕ^2 becomes smaller and $p_\phi^2 \ll p_{\rm C}^2$, the transmission probability is expected to dominate while the bouncing probability becomes smaller and vice versa. Indeed, a more direct dimensional analysis argument is perhaps clearer. Assuming the change in the function $f(\lambda b)$ in the region of interest is order unity [which is approximately correct for a continuous function unless one dramatically tunes $f(\lambda b)$], then the criterion of softness is very simple and boils down to the condition that[8]

$$p_\phi^2 \lesssim \ell_p^2. \tag{6.16}$$

[8]It is interesting to notice that if we assume that the universe is described by a massless scalar field before the onset of inflation, one can estimate p_ϕ as follows. Using Eq. (5.9) we have

$$\rho \sim \frac{p_\phi^2}{V_0^2 a^6}. \tag{6.15}$$

If we assume that the density of the onset of inflation is $\sim 10^{-5} m_{\rm p}^4$—as is the case, for instance, in the power-law inflationary model [51]—and we take the physical volume of the fiducial set at the onset of inflation to be $\sim 10^2 m_{\rm p}^{-3}$, we obtain $p_\phi^2 \sim 10^{-1} m_{\rm p}^{-2} \sim 10^{-1}\ell_{\rm p}^2$. Note that a fiducial cell with a physical volume of 10^2 Planck will inflate to a size much larger than the observable universe today. For a discussion of the role of V_0 in quantum fluctuations, see [52]. This of course adds an additional dimension to the ambiguity discussion.

C. Violation of the NEC due to inverse volume corrections

The NEC requires that $T_{ab}k^a k^b \geq 0$ for any future directed null vector. In our cosmological setting any matter coupling can be considered a perfect fluid as demanded by isotropy, and thus the NEC reduces to the statement that $\rho + P \geq 0$. For a scalar field model of the type considered here (and independently of the self-interaction potential), this condition is classically given by

$$\rho + P = \frac{p_\phi^2}{16\pi^2 G^2 \gamma^2 v^2}, \tag{6.17}$$

which satisfies the NEC trivially. In the quantum theory the NEC can be violated by the inverse volume corrections introduced by a regularization, for instance, of the class (3.14). As an example we plot the regularization

$$\left[\frac{1}{v^2}\right]_{\text{reg}} = \left(2\left[\frac{1}{\sqrt{v}}\right]_{20} - \left[\frac{1}{\sqrt{v}}\right]_2\right)\left(\left[\frac{1}{\sqrt{v}}\right]_2\right)^3 \tag{6.18}$$

in Fig. 6, where one observes that the NECs are violated near the big bang. Such a possibility (which is again directly related to the ambiguities of the polymer quantization) has a strong dynamical effect. In the special case of a massless scalar field, the previous effect also implies a violation of the weak and strong energy conditions in the matter sector. When translated into the nonrelativistic particle analogy of Sec. II, one observes that the effective potential in the Hamiltonian (3.2) is no longer negative definite. This implies that for a sufficiently low cosmological constant—and under suitable conditions where the function $f(\lambda b)$ plays a role—the universe might bounce through yet another channel due to the repulsive potential produced by the negative energy brought about by the regularization before reaching one of the critical points of $f' = 0$. Once again, this is possible if the initial conditions for the matter fields are sufficiently soft so that the probability of this new channel is activated before the standard kinetic bounce described in Sec. VI A takes place. A simple analysis that evaluates the amount of "kinetic" energy acquired by the universe (in the nonrelativistic particle analogy) as it evolves towards the would-be singularity shows that the condition is

$$\left|\frac{p_\phi}{\ell_p}\right| \lesssim \left|\frac{v_c}{\lambda}\right|, \tag{6.19}$$

where v_c is the value of v that maximizes the regularization $v^{-2}|_{\text{reg}}$ before the NECs are violated (explicitly seen around $v = 20$ in Fig. 6 in this particular example). As v_c can be made large by tuning the inverse volume regularization, the present criterion of softness is weaker than the one for tunneling (6.16).

D. Illustrating examples

1. Inflation induced by ambiguity parameters

In order to illustrate how the ambiguities of loop quantum cosmology can actually affect the physics in a nontrivial manner, in this section we show that the modifications introduced by the function $f(\lambda b)$ can, for instance, drive inflation for a large number of e-folds in a way that is weakly dependent on the matter content and dynamics and basically due to the dynamical modifications brought about by the "holonomy corrections" in $f(\lambda b)$. We illustrate this with two simple models: first with a model of a universe filled with thermal radiation and second with a model of inflation with a scalar field with potential $U(\phi) = \lambda\phi^4/2$. The first example shows that one can get many e-folds of inflation without an inflaton. The second contains a scalar field, but the inflation will be

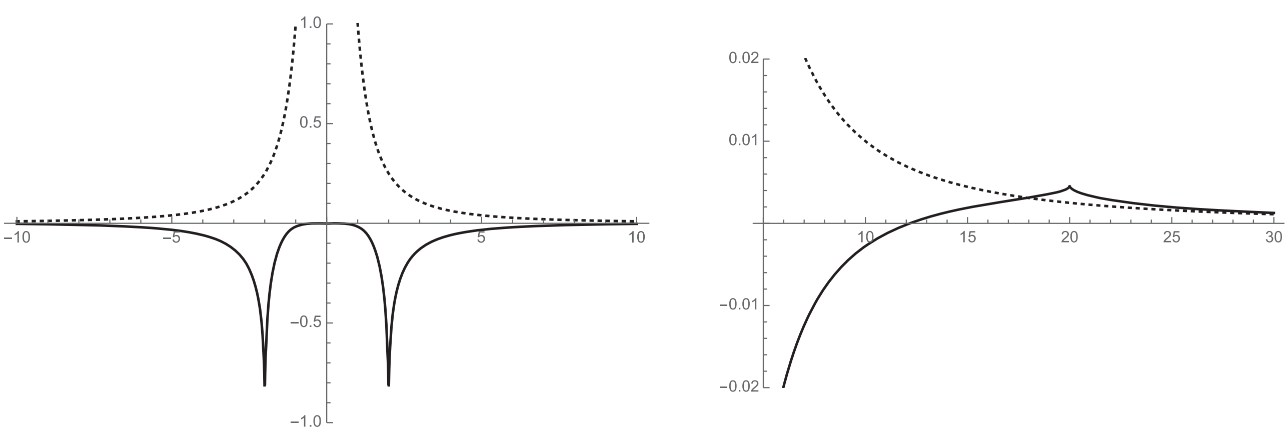

FIG. 6. Regularization of the function $1/v^2$. The classical function corresponds to the dotted line. The regularization shown here violates the positivity in a range around $v = 0$ and coincides, in the IR, with the classical function, as the plot on the right illustrates. This leads from Eq. (6.17) to violations of the NEC that, when considered in the Hamiltonian, produce a different type of bounce for suitable initial conditions. The plot represents the regularization given in (6.18).

driven by the effects of $f(\lambda b)$. As a consequence, the phenomenology observable in the CMB fluctuations can be tuned, as we will show, by judiciously choosing the latter function. Thus, let us consider a function $f(\lambda b)$ such that

$$f'(\lambda b)^2 = \begin{cases} 1 & b < b_c \\ \frac{3H_0^2}{8\pi G}\frac{1}{\rho[\lambda b]} & b > b_c, \end{cases} \tag{6.20}$$

where from (5.1) we have

$$\rho[\lambda b] = \bar{\rho} f(\lambda b)^2, \tag{6.21}$$

and continuity of $f(\lambda b)$ requires

$$\rho[\lambda b_c] = \frac{8\pi G}{3H_0^2} \equiv \rho_c, \tag{6.22}$$

with ρ_c a critical density depending on the choice of H_0. A solution of the differential equation (6.20) is given by

$$f(\lambda b) = \begin{cases} \lambda b & b < b_c \\ \sqrt{2\gamma\lambda^2 H_0(b - b_c) + \lambda^2 b_c^2} & b > b_c. \end{cases} \tag{6.23}$$

This choice of $f(\lambda b)$ produces the standard Friedmann equation for $\rho \leq \rho_c$, while it produces a Friedmann equation with a constant Hubble rate H_0 (de Sitter inflation) for $\rho \geq \rho_c$ regardless of the equations of state of matter. The matter equations of state only control [via (5.16)] how long the universe will remain in the inflationary phase. We construct two explicit examples in what follows.

2. Pure radiation inflationary model

The first model consists of a universe filled with radiation $\rho = 3P$. In this case, from (5.16) one has that

$$\rho = \rho_{\rm in}\frac{a_{\rm in}^4}{a^4}. \tag{6.24}$$

Assuming the initial value of $\rho_{\rm in} = m_p^4$ (Planck density) and setting $\rho_c = 10^{-68}\rho_{\rm in}$ in (6.22) to the electroweak transition density,[9] we see that inflation can be sustained as long as

$$\frac{a_{\rm in}^4}{a^4} \geq 10^{-68}, \tag{6.25}$$

in other words, for a number of e-folds of about

$$\mathcal{N}_{\rm rad} = 17\log(10) \approx 39. \tag{6.26}$$

[9]The electroweak transition energy scale is $E_{\rm ew} \approx 100$ GeV, which corresponds to $E_{\rm ew} \approx 10^{-17} m_p$.

Using a massless scalar field (which is an often-used example) with the equation of state $P = \rho$, one has

$$\rho = \rho_{\rm in}\frac{a_{\rm in}^6}{a^6}, \tag{6.27}$$

and for ρ_c we get $\mathcal{N}_\phi = \log[10]68/6 \approx 26$, which is still a considerable number.

E. Inflation with a scalar field

It is also possible to design a model without an inflaton using only the matter content of the standard model of particle physics where inflation is driven by polymer corrections. The model is consistent with the observed fluctuations in the CMB if the usual paradigm, where quantum fluctuations of the Higgs [with potential $U(\phi) = \frac{\alpha}{2}\phi^4$] are responsible for the generation of inhomogeneities, is used. More precisely, starting from the Klein-Gordon equation for the Higgs zero mode,

$$\ddot{\phi} + 3H\dot{\phi} + 2\alpha\phi^3 = 0, \tag{6.28}$$

and using the standard terminal velocity approximation ($\frac{\ddot{\phi}}{H\dot{\phi}} \ll 1$), the solution of (6.28) is given by

$$\phi(t) = \frac{\phi_0}{\sqrt{1 + \frac{4}{3}\alpha\frac{\phi_0^2}{H_0^2}H_0 t}} \quad \text{or} \quad \phi(\mathcal{N}) = \frac{\phi_0}{\sqrt{1 + \frac{4}{3}\alpha\frac{\phi_0^2}{H_0^2}\mathcal{N}}}, \tag{6.29}$$

where we introduced the number of e-folds $\mathcal{N} = \log(a) \approx H_0 t$. Now, using $\rho = \frac{\dot{\phi}^2}{2} + \frac{\alpha}{2}\phi^4$ and Eq. (6.29) we obtain

$$\rho(\mathcal{N}) = \frac{\alpha}{2}\frac{\phi_0^4}{\left[1 + \frac{4}{3}\alpha\frac{\phi_0^2}{H_0^2}\mathcal{N}\right]^2}\left(\frac{2\alpha}{3}\frac{\frac{\phi_0^2}{H_0^2}}{\left[1 + \frac{4}{3}\alpha\frac{\phi_0^2}{H_0^2}\mathcal{N}\right]} + 1\right), \tag{6.30}$$

where ϕ_0 is the initial value of the scalar field. Let us assume that we want

$$\mathcal{N} = 50. \tag{6.31}$$

Then, the previous expression must satisfy the condition (6.22). Introducing the variables $y \equiv m_p/\phi_0$ and $x \equiv \phi_0/H_0$, we can write it as

$$\frac{3y^2}{8\pi} = \frac{\alpha}{2}\frac{x^2}{\left[1 + \frac{200\alpha}{3}x^2\right]^2}\left(\frac{2\alpha}{3}\frac{x^2}{\left[1 + \frac{200\alpha}{3}x^2\right]} + 1\right), \tag{6.32}$$

which imposes some algebraic restrictions on the initial value ϕ_0 and the Hubble rate H_0. We can solve this numerically. For instance, we find the solutions $\phi_0 \approx 10 m_p$ and $H_0 \approx m_p$ if we choose $\alpha = 10^{-3}$ (for such a small coupling we could solve the previous constraint analytically, neglecting the subleading corrections in α, but this is not really important here as we only want to give an example). At the end of inflation $\phi_{\rm end} \approx 9.7 m_p$, and the reheating phase could start as in the usual approaches such as those of chaotic inflation. This example is perhaps more suitable for our point, as here the densities remain Planckian during the inflationary phase; thus, our deviations from general relativity can be more safely attributed to "quantum gravity" effects. This is in contrast to the previous example where densities decreased to almost standard particle physics densities during the anomalous expansion era. One could investigate the mechanism of structure formation. The point of our example is to show the intrinsic discretional nature of these models, which precludes the possibility to actually use them for such predictions.

VII. CONCLUSIONS

We have investigated regularization ambiguities associated with the so-called polymerization process imposed when quantizing cosmological models using the loop quantum cosmology framework. We showed that quantitative predictability is compromised by the strong dependence on free parameters. As evoked in the Introduction, such ambiguities are expected on general grounds due to the perturbative nonrenormalizable character of general relativity. Nonperturbative and background-independent methods might pave the way towards a UV completion of quantum gravity. Yet it seems clear that these methods can only be reliable if field theoretical degrees of freedom are suitably taken into account. It is too naive to expect that a simple model with finitely many degrees of freedom could shed nontrivial light on such a central issue in quantum gravity.

Minisuperspace models are still interesting as toy models, where different scenarios can be put to the test in a calculable framework. We have seen that these models offer some qualitative features that are robust and independent of the polymerization choice. Among these, one finds the well-defined quantum evolution across of the big bang, which can also be recovered at the level of effective dynamical equations valid for suitable semiclassical states. Thanks to the fact that our quantum dynamics could be explicitly solved, we were able to exhibit the existence of new channels (tunneling) for the transition across the big bang, which are not apparent at the level of the effective dynamical equations. This was possible due to the use of unimodular quantum cosmology; however, it is easy to understand that these features hold true in the standard formulation.

An important feature of the quantum dynamics is that it allows for the evolution of a semiclassical state representing (say) a contracting universe into a superposition of expanding universes after the big bang. Such states (as those represented in Fig. 2–4)—which are clearly nonsemiclassical—make apparent an old challenge that cannot be ignored in quantum cosmology and quantum gravity altogether: namely, how to interpret the quantum theory in a genuinely closed system without exterior observers. Perhaps the simplicity of the model can offer an arena where possible interpretations can be discussed.

The richness of these models should be relevant for the discussion of conceptual and qualitative issues in quantum gravity: for instance, in the discussion of unitarity in the context of the black hole information puzzle (where some initial studies have been performed [43,44]) or in the context of gravitational collapse where the new tunneling modes discussed here could be simplified toy models relevant to investigate the black to white hole transition paradigm of [53–57]. The landscape of models is certainly larger than the one we have explored here. In addition to the holonomy corrections where we mostly focused our discussion, we have mentioned the inverse volume corrections. There are also factor ordering ambiguities and dynamical ambiguities related to the way in which the passage from the so-called μ_0 to $\bar{\mu}$ is performed. All of these factors have an impact on the dynamical predictions of these models. We focused on holonomy corrections because they form an easily identifiable and manageable infinite dimensional subclass.

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APPENDIX: SOME PROPERTIES OF GAUSSIAN STATES IN LQC

The work of Willis and Taveras [31,59] shows that one can approximate the quantum dynamics of loop quantum cosmology by effective classical equations when using suitable semiclassical states defined in terms of Gaussian states. However, their analysis does not include the type of generalized regularizations studied in this paper. In this section we show that the effective dynamics approximation continues to make sense for arbitrary regularizations of the quantum Hamiltonian as defined in (3.2).

Let us specialize to a natural choice of semiclassical states (customarily used in the literature when studying the issues involved here [31,59]). We choose a state $|\Psi\rangle \in \mathscr{H}_{lqc} \otimes \mathscr{H}_{\phi}$ as a Gaussian state given by

$$|\Psi\rangle = \sum_{v_n \in \Gamma_\lambda} \int_{\mathbb{R}} dp \Psi_{v_0,b_0}(v_n) \Phi_{p_0,\phi_0}(p) |v_n, p\rangle \quad \text{(A1)}$$

where one uses the basis eigenstates of v and p, respectively, with the (physical) inner product

$$\langle v_m, p' | v_n, p\rangle = \delta_{n,m} \delta(p, p'). \quad \text{(A2)}$$

Here, the wave function

$$\Psi_{v_0,b_0}(v) = \sqrt{\frac{\lambda \sigma_b}{\sqrt{\pi}}} e^{-\frac{\sigma_b^2}{2}(v-v_0)^2} e^{ib_0(v-v_0)} \quad \text{(A3)}$$

is peaked at the geometry phase space point (v_0, b_0), and the wave function

$$\Phi_{p_0,\phi_0}(p) = \sqrt{\frac{\sigma_\phi}{\sqrt{\pi}}} e^{-\frac{\sigma_\phi^2}{2}(p-p_0)^2} e^{i\phi_0(p-p_0)} \quad \text{(A4)}$$

represents a semiclassical state peaked at the point (ϕ_0, p_0) of the scalar field phase space. In the previous expressions Γ_λ denotes a regular lattice with lattice spacing λ that identifies the so-called superselected sectors of the quantum geometry Hilbert space (for a discussion of the nature of such choices, see [43,44] and references therein).

1. Equivalence between calculations using the discrete or continuum inner products

The following remark gives the means to translate expressions involving discrete sums in the loop quantum cosmology inner product to the more familiar continuous integrals of the Schrödinger representation.

Remark 1. For any operator $O(b,p) = \sum_k o_k(p) e^{ib\lambda k}$ and Gaussian semiclassical states as in (A1), one has that

$$\boxed{\langle O(b,p)\rangle \equiv \langle \Psi | O(b,p) | \Psi\rangle.} \quad \text{(A5)}$$

Proof.—By linearity, it is enough to prove the previous statement for the operator $e^{ikb\lambda}$ for arbitrary k. One has

$$\begin{aligned} \langle \Psi | e^{ikb\lambda} | \Psi\rangle &= \frac{\lambda \sigma_b}{\sqrt{\pi}} \sum_{n,m} e^{-\frac{\sigma_b^2}{2}(\lambda n - v_0)^2} e^{-ib_0(\lambda n - v_0)} e^{-\frac{\sigma_b^2}{2}(\lambda m - v_0)^2} e^{ib_0(\lambda m - v_0)} \langle n | m-k\rangle \\ &= \frac{\lambda \sigma_b e^{i2b_0\lambda k}}{\sqrt{\pi}} \sum_m e^{-\frac{\sigma_b^2}{2}(\lambda m - \lambda k - v_0)^2} e^{-\frac{\sigma_b^2}{2}(\lambda m - v_0)^2} \\ &= \frac{\lambda \sigma_b e^{ib_0\lambda k}}{\sqrt{\pi}} e^{-\frac{1}{4}\sigma_b^2 \lambda^2 k^2} \sum_m e^{-\sigma_b^2(\lambda m - v_0 - \lambda\frac{k}{2})^2} = \frac{\sigma_b e^{ib_0\lambda k}}{\sqrt{\pi}} e^{-\frac{1}{4}\sigma_b^2\lambda^2 k^2} \vartheta_3\left[-\frac{\pi}{2}\left(k + 2\frac{v_0}{\lambda}\right); e^{-\frac{\pi^2}{\lambda^2 \sigma_b^2}}\right] \\ &= e^{ib_0\lambda k} e^{-\frac{1}{4}\sigma_b^2 \lambda^2 k^2}\left(1 + \mathscr{O}\left(e^{-\frac{\pi^2}{\lambda^2\sigma_b^2}}\right)\right), \end{aligned} \quad \text{(A6)}$$

where

$$\vartheta_3[u;q] \equiv 1 + 2\sum_{n=1}^{\infty} q^{n^2} \cos[2nu]. \quad \text{(A7)}$$

In the first line we used the definition of the states, (A1) and (4.1), and then we rearranged the sums, completing squares to arrive at the final result.

Corollary 1. For any operator $O(\lambda b, p) = \sum_k o_k(p) e^{ikb\lambda}$ and Gaussian semiclassical states as in (A1), one has

$$\frac{d\langle \Psi | O(\lambda b, p)\Psi\rangle}{d(\lambda b_0)} = \left\langle \frac{dO(\lambda b, p)}{d(\lambda b)}\right\rangle. \quad \text{(A8)}$$

The proof of the previous statement follows directly from (A6). ■

Corollary 2. For any operator $f(\lambda b) = \sum_k f_k e^{ikb\lambda}$ and Gaussian semiclassical states as in (A1), one has

$$\langle f(b)^2\rangle - \langle f(b)\rangle^2 = 2f'(\lambda b_0)^2 \lambda^2 \sigma_b^2 + \mathscr{O}(\lambda^4 \sigma_b^4). \quad \text{(A9)}$$

Proof.—From Remark 1, we have

$$\langle f(\lambda b)\rangle = f(\lambda b_0) + \frac{1}{4} f''(\lambda b_0) \lambda^2 \sigma_b^2 + \mathscr{O}(\lambda^4 \sigma_b^4). \quad \text{(A10)}$$

The present statement follows from the previous equation when applied to $O(b) = f^2(b)$ and $O(b) = f(b)$, respectively, and by replacing the result in the expression of the fluctuation. ■

Corollary 3. The previous two results imply that

$$\frac{d\langle f(\lambda b)^2\rangle}{db_0} = 2\frac{d\langle f(\lambda b)\rangle}{db_0}\langle f(\lambda b)\rangle + \mathcal{O}(\lambda^2\sigma^2). \tag{A11}$$

2. Generating function and the expectation value of operators depending on the volume

Remark 2. For any operator $O(b,p) = \sum_k o_k(p)e^{ib\lambda k}$ and Gaussian semiclassical states as in (A1), one has the generating function on the left,

$$\boxed{\frac{\langle\Psi|e^{\mathcal{J}(v-v_0)}O(b,p)|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_k o_k(p)e^{ib_0k}e^{-\frac{1}{4}\sigma_b^2\lambda^2k^2+\frac{\mathcal{J}^2}{4\sigma_b^2}-\mathcal{J}\lambda\frac{k}{2}} + \left(1+\mathcal{O}\left(e^{-\frac{\pi^2}{\lambda^2\sigma_b^2}}\right)\right)}, \tag{A12}$$

and the generating function on the right,

$$\boxed{\frac{\langle\Psi|O(b,p)e^{\mathcal{J}(v-v_0)}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_k o_k(p)e^{ib_0k}e^{-\frac{1}{4}\sigma_b^2\lambda^2k^2+\frac{\mathcal{J}^2}{4\sigma_b^2}+\mathcal{J}\lambda\frac{k}{2}} + \left(1+\mathcal{O}\left(e^{-\frac{\pi^2}{\lambda^2\sigma_b^2}}\right)\right)}. \tag{A13}$$

Proof.—Consider

$$\begin{aligned}\langle\Psi|e^{ikb\lambda}e^{\mathcal{J}(v-v_0)}|\Psi\rangle &= \frac{\lambda\sigma_b}{\sqrt{\pi}}\sum_{n,m}e^{-\frac{\sigma_b^2}{2}(\lambda n-v_0)^2}e^{-ib_0(\lambda n-v_0)}e^{-\frac{\sigma_b^2}{2}(\lambda m-v_0)^2}e^{ib_0(\lambda m-v_0)}e^{\mathcal{J}(\lambda m-v_0)}\langle n|m-k\rangle \\ &= e^{ib_0k}e^{-\frac{1}{4}\sigma_b^2\lambda^2k^2+\frac{\mathcal{J}^2}{4\sigma_b^2}+\mathcal{J}\lambda\frac{k}{2}}\left(1+\mathcal{O}\left(e^{-\frac{\pi^2}{\lambda^2\sigma_b^2}}\right)\right),\end{aligned} \tag{A14}$$

where in the second line we completed the square and performed the Gaussian integration. Equation (A13) follows from the last line. A similar manipulation gives (A12). ■

3. Some statements about the truncation of the Fourier expansion

Given a bounded square integrable function $f(\lambda b)$ of period 2π, we can write

$$f(\lambda b) = \sum_{n\in\mathbb{Z}} a_n e^{in\lambda b}, \tag{A15}$$

with the coefficients a_n given by

$$a_n = \frac{1}{2\pi}\int_0^{2\pi} f(\lambda b)e^{-in\lambda b}d(\lambda b), \tag{A16}$$

which can be bounded by

$$|a_n| \leq f_{\max}, \tag{A17}$$

where $f_{\max} \equiv \max|f(\lambda b)|$. Let us define the truncated function as

$$f_N(\lambda b) = \sum_{n=-N}^{+N} a_n e^{in\lambda b}. \tag{A18}$$

Remark 3. When evaluated on Gaussian states (A1), one has that

$$\begin{aligned}&|\langle f(\lambda b)\rangle - \langle f_N(\lambda b)\rangle| \\ &\quad\leq 2f_{\max}e^{-\sigma_b^2\lambda^2N^2}(1+\mathcal{O}(e^{-\sigma_b^2\lambda^2})).\end{aligned} \tag{A19}$$

Therefore, the expectation value of the full series and the truncation agree extremely well as N grows. We can say the difference between the two will be negligible as long as

$$\boxed{\lambda^2\sigma_b^2N^2 > 1}. \tag{A20}$$

Proof.—It follows from Remark 2 that

$$\begin{aligned}|\langle f(\lambda b)\rangle - \langle f_N(\lambda b)\rangle| &= \left|\sum_{|n|>N} a_n e^{in\lambda b_0} e^{-\sigma_b^2\lambda^2 n^2}\right| \leq 2\sum_{n=N+1}^{+\infty}|a_n|e^{-\sigma_b^2\lambda^2 n^2} = 2e^{-\sigma_b^2\lambda^2 N^2}\sum_{n=N+1}^{+\infty}|a_n|e^{-\sigma_b^2\lambda^2(n^2-N^2)} \\ &\leq 2e^{-\sigma_b^2\lambda^2 N^2}\sum_{n=N+1}^{+\infty}|a_n|e^{-\sigma_b^2\lambda^2(n-N)^2} = 2e^{-\sigma_b^2\lambda^2 N^2}\sum_{m=1}^{+\infty}|a_{m+N}|e^{-\sigma_b^2\lambda^2 m^2} \\ &\leq 2f_{\max}e^{-\sigma_b^2\lambda^2 N^2}(1+\mathcal{O}(e^{-\sigma_b^2\lambda^2})). \end{aligned} \tag{A21}$$

■

Corollary 4. For a given function $f(\lambda b)$ and Gaussian states (A1), we have

$$\langle f_N(\lambda b)\rangle \approx f(\lambda b_0) \tag{A22}$$

as long as

$$\boxed{\frac{1}{N^2} < \lambda^2\sigma_b^2 < \left|\frac{4f(\lambda b_0)}{f''(\lambda b_0)}\right|} \tag{A23}$$

which can be achieved for sufficiently large N. We therefore arrive at the conclusion that for any arbitrary function $f(\lambda b)$ we can find N and σ_p such that the Gaussian expectation value agrees to the desired accuracy with the function of our choice satisfying the minimal requirement (3.3).

Remark 4. remyy For arbitrary operators $O(\beta b)$, the following time evolution rule holds:

$$\begin{aligned}\frac{d\langle O(\beta b)\rangle}{ds} &\equiv -i\langle[O(\beta b),\mathcal{H}]\rangle \\ &= \frac{V_0}{4\pi G\gamma}\frac{\langle p_\phi^2\rangle}{\pi G\gamma v_0^3}\frac{d\langle O(\beta b)\rangle}{db_0} + \mathcal{O}\left(\frac{\beta^2}{v_0^4}\right),\end{aligned} \tag{A24}$$

where one needs to assume that $v_0 \gg \sigma_b$ and $v_0 \gg N$.

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