Quantum singularities in Hořava-Lifshitz cosmology

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The recently proposed Hořava-Lifshitz theory of gravity is analyzed from the quantum cosmology point of view. By employing usual quantum cosmology techniques, we study the quantum Friedmann-Lemaître-Robertson-Walker universe filled with radiation in the context of Hořava-Lifshitz gravity. We find that this universe is quantum mechanically nonsingular in two different ways: the expectation value of the scale factor $\langle a\rangle(t)$ never vanishes and, if we abandon the detailed balance condition suggested by Hořava, the quantum dynamics of the universe is uniquely determined by the initial wave packet and no boundary condition at $a = 0$ is necessary.

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I. INTRODUCTION

In 2009, Hořava proposed a new theory of gravitation [1] based on an anisotropic scaling of space $\mathbf{x}$ and time t coordinates. The resulting theory, since then dubbed Hořava-Lifshitz (HL) gravity, has proved to be power-countable renormalizable. One of its key points is that, even though it does not exhibit relativistic invariance at short distances, general relativity (GR) is indeed recovered for low-energy limits. Some interesting consequences of this theory include the existence of nonsingular bouncing universes [2–4] and the possibility that it may represent an alternative to inflation, since it might solve the flatness and horizon problem and generate scale-invariant perturbations for the early universe without the need for exponential expansion [5–7].

Due to the asymmetry of space and time in the HL gravity, its natural framework is the Arnowitt-Deser-Misner (ADM) formalism [8], where the spacetime metric $g_{\mu\nu}(t, \mathbf{x})$ is decomposed as usual in terms of the three-dimensional metric $h_{ij}(t, \mathbf{x})$ of the spatial slices of constant t, the lapse function $N(t, \mathbf{x})$, and the shift vector $N^i(t, \mathbf{x})$. In his original work, Hořava made an important assumption about the lapse function to simplify the HL gravitational action, the so-called "projectability condition", namely $N \equiv N(t)$. There are, nevertheless, extended models where this condition is relaxed. Projectable theories give rise to a unique integrated Hamiltonian constraint, leading to great complications when compared with GR. The so-called nonprojectable theories, on the other hand, typically give rise to a local Hamiltonian constraint, as in GR. Healthy nonprojectable extensions of the original HL gravitational action are discussed in detail in Ref. [9]. Fortunately, since Friedmann-Lemaître-Robertson-Walker (FLRW) spacetimes are homogeneous and isotropic, the spatial integral can be dropped from the integrated Hamiltonian constraint in our case [10,11], yielding a true local constraint even for the projectable case. For our purposes here, it suffices to consider the simplest HL projectable theory in an FLRW spacetime. We notice that a modified $F(R)$ HL theory in an FLRW spacetime has been recently considered in Ref. [12], leading to very interesting results regarding the possible unification between primordial inflation and dark energy. Another important assumption originally introduced by Horava is the principle of "detailed balance". This condition, which states that the potential in the gravitation action follows from the gradient flow generated by a three-dimensional action, reduces the number of independent coupling constants. Recently, it has became clear that the detailed balance condition can be also relaxed [10,13–16]. In particular, in Refs. [14,15] the dynamical role and the consequences for the matter couplings of the detailed balance condition in classical cosmology are detailed. In this paper we will abandon the detailed balance condition since, as we will show, it gives rise to the most interesting quantum universes. The limit where this condition can be recovered will also be discussed.

There have been many attempts to incorporate quantum mechanics into GR. One of the first ones was quantum cosmology. In quantum cosmology, we work with the Hamiltonian (ADM) formulation of GR, using Dirac's algorithm [17] of quantization, i.e., the substitution $\pi_q \to -i\delta/\delta q$, where π_q is the canonical momentum associated with the variable q (which can be one of the three canonical variables in GR, h_{ij}, N or N^i), and the imposition that the first-class constraints of the theory should annihilate the wave function of the spacetime. GR has four constraints: three of them simply tell us that the wave function of the spacetime depends only on the intrinsic geometry of the spatial slices in the ADM decomposition, while the last one is a dynamical constraint which gives the dynamical equation of quantum cosmology, the so-called Wheeler-DeWitt equation [18]. The wave function is *a priori* defined on the space of all 3-metrics—called superspace—which are in general very intricate infinite-dimensional spaces. However, we can take advantage of the symmetries of a homogeneous universe to freeze out all but a finite number

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of degrees of freedom of the metric, and then quantize the remaining ones. These models are known as minisuperspace models. Quantum cosmology in FLRW minisuperspace filled with a perfect fluid has been shown to be viable and interesting in the sense that the initial big bang singularity is not present in such a model since $\langle a\rangle(t) \neq 0$ for all times, and the classical behavior of the universe is recovered for large times [19,20]. Moreover, in this class of models a certain evolution parameter of the fluid gives us a measure of time, and one can investigate the evolution of the scale factor as the fluid evolves.

For static spacetimes, Horowitz and Marolf [21] found an original way of classifying a spacetime as quantum mechanically nonsingular. In their work, a spacetime is said to be quantum mechanically nonsingular if the evolution of quantum particles in the classical background is uniquely determined by the initial wave packet, i.e., no boundary conditions at the classical singular points are necessary. This is equivalent to saying that the spatial part of the wave equation is essentially a self-adjoint operator, i.e., it has a unique self-adjoint extension (for a review of the mathematical framework necessary to define quantum singularities in static spacetimes, see Ref. [22]). In the GR context, the quantization of the FLRW minisuperspace filled with a perfect fluid does require a boundary condition at $a = 0$ in order to assure the self-adjointness of the Wheeler-DeWitt equation, which, on the other hand, is necessary to guarantee a unitary time evolution. Mathematically, the Hamiltonian operator corresponding to the evolution equation of the universe is not essentially self-adjoint. In this way the quantum dynamics of the universe is not unique since we do not know, in principle, which boundary condition we must apply at the initial singularity. However, as we will see later, it is possible to find quantum cosmologies in the HL gravity context for which the quantum evolution of the universe is unique, and no boundary condition for the wave function is necessary.

In this paper we will apply the machinery of quantum cosmology to the HL theory of gravity. In particular, we will investigate the necessity of initial boundary conditions for the Wheeler-DeWitt equation and the behavior of the universe by examining the time evolution of the expectation value of the scale factor. A certain evolution parameter of the radiation filling the universe will play the role of the time coordinate. The content of the universe will be introduced in the gravitational action via the Schutz formalism [23,24], demanding the recovery of the usual GR formulation in the low-energy [25]. The paper is organized as follows. Sections II, III, and IV present brief reviews of the results we need and the main definitions about quantum singularities, the HL theory of gravity, and the usual quantum cosmology in the GR context, respectively. Our main results are presented in Secs. V and VI. The last section is devoted to some concluding remarks.

II. QUANTUM SINGULARITIES

Typical solutions of the Einstein field equations are known to exhibit singularities. They can be classified as [26]: quasiregular singularities, where the observer feels no physical quantity diverging, except at the moment when its worldline reaches the singularity (for instance, the conical singularity of a cosmic string); scalar curvature singularities, where every observer approaching the singularity experiences diverging tidal forces (for example, the singularity inside a black hole and, more important in the present context, the big bang singularity in FLRW cosmology); nonscalar singularities, where there are some curves in which the observers experience unbounded tidal forces (for example, whimper cosmologies). It is well known [27] that under very reasonable conditions (the energy conditions), which basically state that gravity must be attractive, singularities are inevitable in GR. In this way, cosmological models with nonexotic fluids, as radiation or dust, typically present an initial singularity, known as the big bang singularity. Since we cannot escape this fact in GR, we hope that the quantum theory of gravitation will solve this issue, guiding us in how to deal with the singularities, or even excluding them entirely. Unfortunately, we do not yet have such a theory. However, there is much evidence that this theory would actually solve this problem. This evidence comes with the introduction of quantum mechanics in GR in many different ways. In this paper we will highlight two distinct approaches.

The first approach is quantum field theory in curved spacetimes. In this framework, we analyze the behavior of quantum particles (or fields) in a classical curved background, which we assume to be a regular solution of the Einstein field equations. We adopt Horowitz and Marolf's definitions [21]. In their work, they analyze the behavior of a scalar particle in singular static spacetimes possessing a timelike Killing vector field ξ^μ. In such spacetimes, the wave equation can be separated into

$$\frac{\partial^2\Psi}{\partial t^2} = -A\Psi, \tag{1}$$

where $A = -VD^i(VD_i) + V^2M^2$ and $V = -\xi^\mu\xi_\mu$, with D_i being the spatial covariant derivative in a static slice Σ not containing the singularity. In principle, the domain $\mathcal{D}(A)$ of the operator A is not known, so we choose as a first attempt $\mathcal{D}(A) = C_0^\infty(\Sigma)$. In this way, our operator is symmetric and positive definite. However, this domain is unnecessarily small; in other words, the conditions on the functions are so restrictive that the operator A is not self-adjoint. Its adjoint operator A^* has a much larger domain $\mathcal{D}(\mathcal{A}^*) = \{\Psi \in L^2(\Sigma): A\Psi \in L^2(\Sigma)\}$. It is important to notice that we have chosen $L^2(\Sigma)$ as the Hilbert space of our quantum theory (for a discussion about this point see Ref. [22]). We must relax the conditions on the allowed functions in order to extend the domain of A in such a way that $\mathcal{D}(A^*) \to \mathcal{D}(A)$. If the extended operator is unique,

A is said to be essentially self-adjoint, and its extension is given by $(\bar{A}, \mathcal{D}(\bar{A}))$, where $\bar{A}$ is the closure of A (for more details see Ref. [28]). The time evolution of the particle will then be given by

$$\Psi(t) = \exp(-it\bar{A}^{1/2})\Psi(0), \tag{2}$$

and the spacetime is said to be quantum mechanically nonsingular. However, if the extension is not unique, i.e., if there exists infinitely many extensions A_α, with α being a parameter such that to each α there corresponds one boundary condition at the singular point, then we have a different time evolution,

$$\Psi_\alpha(t) = \exp(-itA_\alpha^{1/2})\Psi(0), \tag{3}$$

for each α. In this case, the spacetime is said to be quantum mechanically singular. Similar to the classical case, when a spacetime is quantum mechanically singular extra information (a boundary condition) must be given in order to obtain the time evolution. In particular, in GR we need to tell what happens to the particle when it reaches the singularity.

The second approach we exploit here is quantum cosmology in minisuperspaces. In this framework, we consider a few degrees of freedom of the system (the rest are assumed to be frozen) and quantize the constraints of the theory via Dirac's algorithm. We impose $[a, p_a] = i$ (in units where $\hbar = 1$), where a is the scale factor of FLRW models, and $[T, p_T] = i$, where T is a parameter associated with the evolution of the fluid filling the universe. In this way, we obtain the Wheeler-DeWitt equation of the universe, which, as we will see, is a Schrödinger-like equation from which we can define an internal product between two solutions and, therefore, evaluate expectation values of observables. In this context, we define the universe as nonsingular if $\langle a\rangle(t) \neq 0$ for all times. Since the operator $\hat{a}$ is positive in $L^2(0,\infty)$, we will have $\langle a\rangle(t) = 0$ if the wave function representing the universe is sharply peaked at $a = 0$. Note that this criterion is different from that originally stated by DeWitt, which says that the universe is quantum mechanically nonsingular if $\Psi(a = 0, t) \neq 0 \forall\ t$. In fact, it was shown that this criterion is not enough to prevent singularities in quantum cosmological models [29].

The two classifications of quantum singularities described above belong to completely different frameworks, but we can apply the mathematical machinery used in static spacetimes in order to decide if the evolution of a wave packet governed by the Wheeler-Dewitt equation is unique in a given quantum cosmology scenario.

III. HL GRAVITY

In order to introduce the HL theory of gravity, let us first introduce the decomposition of the metric in the ADM form,

$$ds^2 = -N^2c^2dt^2 + h_{ij}(dx^i - N^i dt)(dx^j - N^j dt), \tag{4}$$

and then let us postulate that the dimensions of space and time are (in units of momentum) $[dx^i] = -1$ and $[dt] = -3$. This assumption assures that the theory is power-countable renormalizable in four dimensions. In these units, we have $[N] = [h_{ij}] = 0$, while $[N^i] = 2$, leading to $[ds^2] = -2$. Notice that the volume element, defined by

$$dV_4 = N\sqrt{h}d^3\mathbf{x}dt, \tag{5}$$

has dimension $[dV_4] = -6$.

The extrinsic curvature tensor, which measures how the spatial slices in the ADM decomposition of spacetime curve with respect to external observers, is defined by

$$K_{ij} = \frac{1}{2N}\left(\frac{\partial h_{ij}}{\partial t} - \nabla_{(i}N_{j)}\right). \tag{6}$$

It is easy to see that it has dimension $[K_{ij}] = 3$. The most general term involving the extrinsic curvature tensor which is invariant under the group of diffeomorphisms of the spatial slices will define the kinetic term in the action. This term depends on two coupling constants α and λ, and is given by

$$S_K = \alpha\int dtd^3\mathbf{x}\sqrt{h}N(K_{ij}K^{ij} - \lambda K^2). \tag{7}$$

Note that $[\alpha] = 0$, i.e., α is a dimensionless constant. This is the reason why we made the choice $[dt] = -3$.

The potential term for the gravitational action is given by

$$S_V = -\int dtd^3\mathbf{x}\sqrt{h}NV[h_{ij}], \tag{8}$$

where $V[h_{ij}]$ is built out of the spatial metric and its spatial derivatives. Since $[dV_4] = -6$, we must have $[V[h_{ij}]] = 6$ in order to assure that S_V is a scalar. The most general action (without the detailed balance condition) containing terms with dimensions less than or equal to 6 is given by (for more details see Ref. [10])

$$S_{\rm HL} = S_K + S_V, \tag{9}$$

where

$$\begin{aligned} V[h_{ij}] = {}& g_0\zeta^6 + g_1\zeta^4R + g_2\zeta^2R^2 + g_3\zeta^2R_{ij}R^{ij} \\ & + g_4R^3 + g_5R(R_{ij}R^{ij}) + g_6R^i{}_jR^j{}_kR^k{}_i \\ & + g_7R\nabla^2R + g_8\nabla_iR_{jk}\nabla^iR^{jk}. \end{aligned} \tag{10}$$

Here the constant ζ has dimension $[\zeta] = 1$ and ensures that all the coupling g_a are dimensionless. In order to restore the units where $c = 1$, i.e., $[dx] = [dt]$, we need to perform the transformation $dt \to \zeta^{-2}dt$.

Since $[R^i_{jkl}] = 2$, as we go to lower momenta the dominant action is

$$S_{\rm IR} = \int dtd^3\mathbf{x}N\sqrt{h}[\alpha(K_{ij}K^{ij} - \lambda K^2) - g_1\zeta^4 R - g_0\zeta^6]. \tag{11}$$

We can now rescale time and space so that $\alpha = 1$ and $g_1 = -1$, and set $c = \lambda = 1$, leading to

$$S_{\rm IR} = \zeta^2 \int dtd^3\mathbf{x}N\sqrt{h}[(K_{ij}K^{ij} - K^2) + R - g_0\zeta^2]. \tag{12}$$

Note that, by choosing

$$\zeta^2 \equiv \frac{1}{16\pi G}, \qquad \Lambda = \frac{g_0\zeta^2}{2}, \tag{13}$$

we have the usual Einstein-Hilbert action

$$\begin{aligned} S_{\rm GR} &= \frac{1}{16\pi G}\int dtd^3\mathbf{x}N\sqrt{h}(K_{ij}K^{ij} - K^2 + R - 2\Lambda) \\ &= \frac{1}{16\pi G}\int d^4x\sqrt{-{}^{(4)}g}({}^{(4)}R - 2\Lambda), \end{aligned} \tag{14}$$

where ${}^{(4)}g_{\mu\nu}$ and ${}^{(4)}R$ are the spacetime metric and Ricci scalar, respectively.

The full HL action we will consider hereafter is

$$\begin{aligned} S_{\rm HL} = \frac{M_P^2}{2}\int dtd^3\mathbf{x}N\sqrt{h}(K_{ij}K^{ij} - \lambda K^2 + R - 2\Lambda \\ - g2M_P^{-2}R^2 - g_3M_P^{-2}R_{ij}R^{ij} - g_4M_P^{-4}R^3 \\ - g_5M_P^{-4}R(R_{ij}R^{ij}) - g_6M_P^{-4}R^i{}_jR^j{}_kR^k{}_i \\ - g_7M_P^{-4}R\nabla^2R - g_8M_P^{-4}\nabla_iR_{jk}\nabla^iR^{jk}), \end{aligned} \tag{15}$$

where $M_P = 1/\sqrt{8\pi G}$ stands for the Planck mass in $c = 1$, $\hbar = 1$ units.

IV. QUANTUM COSMOLOGY IN GR

In the so-called Schutz formalism [23,24] for the matter content of GR, the four-velocity of a perfect fluid is expressed in terms of six potentials in the form

$$U_\nu = \mu^{-1}(\phi_{,\nu} + \alpha\beta_{,\nu} + \theta S_{,\nu}), \tag{16}$$

where μ and S are, respectively, the specific enthalpy and the specific entropy of the fluid. The potentials α and β are connected with rotations and, hence, they are not present in the FLRW universe due to its symmetry. The potentials ϕ and θ have no clear physical meaning. With the usual normalization

$$U^\nu U_\nu = -1, \tag{17}$$

Schutz showed that the action for the fluid in GR is given by

$$S_f = \int d^4x\sqrt{-g}p, \tag{18}$$

where p is the pressure of the fluid, which is related to the density by the equation of state $p = w\rho$. In this way, the total action for the spacetime filled with a perfect fluid is given by

$$S = \frac{M_P^2}{2}\int d^4x\sqrt{-g}(R - 2\Lambda) + \int d^4x\sqrt{-g}p. \tag{19}$$

Varying the above action with respect to the metric, we get the usual Einstein equations,

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = M_P^{-2}T_{\mu\nu}, \tag{20}$$

with $T_{\mu\nu}$ given by

$$T_{\mu\nu} = (\rho + p)U_\mu U_\nu + pg_{\mu\nu}. \tag{21}$$

For the FLRW universe with metric

$$ds^2 = -N^2dt^2 + a(t)^2\left(\frac{dr^2}{1 - kr^2} + r^2d\Omega^2\right), \tag{22}$$

where $d\Omega^2$ is the metric in the unit sphere and $k = -1, 0, 1$ for the open, flat, and closed universe, respectively, the four velocity of the fluid is given by $U_\mu = N\delta^0_\mu$, so that

$$\mu = (\dot\phi + \theta\dot S)/N. \tag{23}$$

On the other hand, by thermodynamical considerations, Lapchinski and Rubakov [30] found that the expression for the pressure is given in terms of the potentials by

$$\begin{aligned} p &= \frac{w\mu^{1+1/w}}{(1 + w)^{1+1/w}}e^{-S/w} \\ &= \frac{w}{(1 + w)^{1+1/w}}\left(\frac{\dot\phi + \theta\dot S}{N}\right)^{1+1/w}e^{-S/w}. \end{aligned} \tag{24}$$

For the particular case of FLRW universes, we have

$$K_{ij} = \frac{\dot a}{Na}h_{ij}, \qquad R_{ij} = \frac{2k}{a^2}h_{ij}, \tag{25}$$

with $h_{ij} = {\rm diag}(\frac{1}{1-kr^2}, r^2, r^2\sin^2\theta)$, so that the total action is given by (in units where $16\pi G = 1$)

$$\begin{aligned} S &= \int dtd^3\mathbf{x}N\sqrt{h}(K_{ij}K^{ij} - K^2 + R) + \int dtd^3\mathbf{x}N\sqrt{h}p \\ &= \int\frac{r^2\sin\theta}{\sqrt{1 - kr^2}}d^3x\int dt\bigg\{-6\frac{\dot a^2a}{N} + 6kNa \\ &\quad + N^{-1/w}a^3\frac{w}{(1+w)^{1+1/w}}(\dot\phi + \theta\dot S)^{1+1/w}e^{-S/w}\bigg\}. \end{aligned} \tag{26}$$

The spatial integration does not affect the equations of motion, and we have the following canonical momenta associated, respectively, with the dynamical variables a, ϕ and S:

$$p_a = -\frac{12\dot aa}{N}, \qquad p_\phi = \frac{N^{-1/w}a^3}{(1 + w)^{1/w}}(\dot\phi + \theta\dot S)^{1/w}e^{-S/w}, \qquad p_S = \theta p_\phi. \tag{27}$$

The Hamiltonian of the system will be given by

$$H = p_a\dot{a} + p_\phi(\dot{\phi} + \theta\dot{S}) - L, \tag{28}$$

where

$$L = -6\frac{\dot{a}a}{N} + 6kNa + N^{-1/w}a^3\frac{w}{(1+w)^{1+1/w}} \times (\dot{\phi} + \theta\dot{S})^{1+1/w}e^{-S/w}. \tag{29}$$

After a tedious but straightforward calculation, we find

$$H = N\left(-\frac{p_a^2}{24a} - 6ka + p_\phi^{1+w}a^{-3w}e^{-S/w}\right). \tag{30}$$

Since the action does not depend on $\dot{N}$, we conclude that N is actually a Lagrange multiplier of the theory. This is not surprising since the results could not depend on how the spacetime is sliced. Varying the action

$$S = \int dt[p_a\dot{a} + p_\phi(\dot{\phi} + \theta\dot{S}) - H] \tag{31}$$

with respect to N leads to the super-Hamiltonian constraint

$$\mathcal{H} = -\frac{p_a^2}{24a} - 6ka + p_\phi^{1+w}a^{-3w}e^{-S/w} \approx 0. \tag{32}$$

Performing a canonical transformation of the form

$$T = -p_S e^S p_\phi^{-(1+w)}, \qquad p_T = p_\phi^{(1+w)}e^S, \qquad \bar{\phi} = \phi + (1+w)\frac{p_S}{p_\phi}, \qquad \bar{p}_\phi = p_\phi, \tag{33}$$

we get

$$\mathcal{H} = -\frac{p_a^2}{24a} - 6ka + \frac{p_T}{a^{3w}} \approx 0. \tag{34}$$

Now, we proceed with Dirac's algorithm of the quantization of constrained systems by making the substitutions $p_a \to -i\partial/\partial a$, $p_T = -i\partial/\partial T$, and demand that the constraint annihilate the wave function, finding the Schrödinger-Wheeler-DeWitt equation of the universe,

$$\frac{\partial^2\Psi}{\partial a^2} + 144ka^2\Psi + i24a^{1-3w}\frac{\partial\Psi}{\partial t} = 0, \tag{35}$$

with $t = -T$ being the time coordinate in the gauge $N = a^{3w}$, as follows from Hamilton's classical equations of motion [31]. Notice that the above equation is of the form $i\partial\Psi/\partial t = \hat{H}\Psi$. In order for the Hamiltonian operator $\hat{H}$ to be self-adjoint we define the internal product of two wave functions as

$$\langle\Phi, \Psi\rangle = \int_0^\infty a^{1-3w}\Phi^*\Psi da, \tag{36}$$

and impose restrictive boundary conditions at $a = 0$. The simplest ones are the Dirichlet and Neumann conditions:

$$\Psi(0,t) = 0\,(\text{Dirichlet}), \qquad \frac{\partial\Psi(0,t)}{\partial a} = 0\,(\text{Neumann}). \tag{37}$$

As we will see, the situation is qualitatively different in the HL theory of gravity.

V. QUANTUM COSMOLOGY IN HL

The total action we will consider here is

$$S = S_{\rm HL} + \int dt d^3\mathbf{x}N\sqrt{h}p, \tag{38}$$

where $S_{\rm HL}$ is given by Eq. (15). We choose this action basically because the GR action can be recovered in the low-energy limit. Discarding the spatial integration again, we have

$$S = \int dt\Big[-3(3\lambda-1)\frac{\dot{a}^2a}{N} + 6Nka - 2\Lambda a^3 - \frac{12kN}{a}(3g_2+g_3) - \frac{24kN}{a^3}(9g_4+3g_5+g_6) + N^{-1/w}a^3\frac{w}{(1+w)^{1+1/w}}(\dot{\phi}+\theta\dot{S})^{1+1/w}e^{-S/w}\Big]. \tag{39}$$

Let us introduce the following constants (as in Ref. [32]):

$$g_C = 6k, \qquad g_\Lambda = 2\Lambda, \qquad g_r = 12k(3g_2+g_3), \qquad g_S = 24k(9g_4+3g_5+g_6). \tag{40}$$

Now, proceeding as in GR, i.e., defining the momenta corresponding to each one of the dynamical variables and calculating the canonical Hamiltonian, we arrive at

$$\mathcal{H} = -\frac{p_a^2}{12(3\lambda-1)a} - g_Ca + g_\Lambda a^3 + \frac{g_r}{a} + \frac{g_s}{a^3} + \frac{p_T}{a^{3w}} \approx 0. \tag{41}$$

Specializing to the radiation case ($w = 1/3$), we find the Schrödinger-Wheeler-DeWitt equation,

$$\frac{\partial^2\Psi}{\partial a^2} - 12(3\lambda-1)\left(g_Ca^2 - g_\Lambda a^3 - g_r - \frac{g_s}{a^2}\right)\Psi + 12(3\lambda-1)i\frac{\partial\Psi}{\partial t} = 0, \tag{42}$$

again with $t = -T$. Note that g_r shifts just the energy levels, since it is a constant in the potential. However, the term g_s changes the effective potential dramatically. The case $g_s = 0$ corresponds to the detailed balance condition [see Ref. [3] where, with the use of the detailed balance condition, Calcagni obtains an action similar to Eq. (39), but without the term proportional to a^{-3}].

VI. EXACT SOLUTIONS

A. Flat FLRW universe

First, note that if we take a spatially flat universe ($k = 0$) with $\Lambda = 0$, we have the following equation:

$$-\frac{1}{12(3\lambda-1)}\frac{\partial^2\Psi}{\partial a^2} = i\frac{\partial\Psi}{\partial t}, \tag{43}$$

which is a Schrödinger-like equation for a free particle with $\hbar = 1$ and mass $m_\lambda = 6(3\lambda - 1)$, except for the requirement $a > 0$. Let us consider only the case $\lambda > 1/3$. In order to ensure the self-adjointness of the above equation, a boundary condition has to be chosen, as discussed in Sec. III. For the sake of simplicity, we choose the Dirichlet boundary condition. For an initial wave packet of the form

$$\Psi(a,0) = \left(\frac{128\sigma^3}{\pi}\right)^{1/4} a e^{-\sigma a^2}, \tag{44}$$

Eq. (43) can be easily solved using a specific propagator (see Ref. [19]). The result is

$$\Psi(a,t) = \left(\frac{m_\lambda}{m_\lambda + 2it\sigma}\right)^{3/2}\left(\frac{128\sigma^3}{\pi}\right)^{1/4} a \times \exp\left(-\frac{-\sigma m_\lambda^2 a^2}{m_\lambda^2 + 4\sigma^2 t^2}\right)\exp\left(\frac{2itm_\lambda \sigma^2 a^2}{m_\lambda^2 + 4\sigma^2 t^2}\right). \tag{45}$$

We can calculate the expectation value of the operator a through the formula

$$\langle a\rangle(t) = \langle \Psi, a\Psi\rangle = \int_0^\infty a|\Psi(a,t)|^2 = \frac{2}{m_\lambda}\sqrt{\frac{2}{\pi\sigma}}\sqrt{\frac{m_\lambda^2}{4} + \sigma^2 t^2}. \tag{46}$$

Note that if we take $\lambda = 1$, we recover the result obtained in Ref. [19]. Nothing changes in HL theory in a flat FLRW universe in comparison with GR (as in the classical case, see for instance [2]). In particular, $\langle a\rangle(t)$ is nonsingular and $\langle a\rangle(t) \sim t$ as $t \to \infty$, recovering the classical behavior of the universe in the classical limit. Besides, the evolution of the wave packet is given once we choose a particular boundary condition at $a = 0$. Therefore, the evolution of the universe is not unique in the sense stated in Sec. II.

B. Closed FLRW universe

For the spatially closed ($k = 1$) FLRW spacetime, there is an effective potential in the Schrödinger-Wheeler-DeWitt equation of the universe. From Eq. (42), we see that this potential represents a shifted quantum harmonic oscillator with a singular perturbation. Setting the mass and frequency of the harmonic oscillator to be $m_\lambda = 6(3\lambda - 1)$ and $\omega_\lambda = \sqrt{2/(3\lambda - 1)}$, respectively, we have the following Schrödinger-like equation:

$$-\frac{1}{2m_\lambda}\frac{\partial^2\Psi}{\partial a^2} + \left(\frac{1}{2}m_\lambda\omega_\lambda^2 a^2 - g_r - \frac{g_s}{a^2}\right)\Psi = i\frac{\partial\Psi}{\partial t}. \tag{47}$$

First, we will analyze the necessity of a boundary condition at $a = 0$ on this equation. The first step is to separate variables in the form $\Psi(a,t) = \psi(a)e^{-iEt}$, leading to

$$\left[-\frac{d^2}{da^2} + V(a)\right]\psi(a) = 2m_\lambda E\psi(a), \tag{48}$$

with

$$V(a) = m_\lambda^2\omega_\lambda^2 a^2 - 2m_\lambda g_r - (2m_\lambda g_s)/a^2. \tag{49}$$

Following Ref. [28], we say that $V(a)$ is in the limit circle case at infinity and at zero if for all λ, all solutions of

$$\left[-\frac{d^2}{da^2} + V(a)\right]\psi(a) = \lambda\psi(a) \tag{50}$$

are square integrable at infinity and at zero, respectively. If $V(a)$ is not in the limit circle case, it is said to be in the limit point case. We now enunciate the Theorem X.7 from Ref. [28], which gives us a criterion to decide if the Hamiltonian operator $\hat{H} = -d^2/da^2 + V(a)$ is essentially self-adjoint, i.e., if it has a unique self-adjoint extension.

Theorem 1.—Let $V(a)$ be a continuous real-valued function on $(0,\infty)$. Then $\hat{H} = -d^2/da^2 + V(a)$ is essentially self-ajoint if and only if $V(a)$ is in the limit point case at both zero and infinity.

We now need a criterion to decide if $\hat{H}$ is in the limit point or limit circle case at zero and infinity. We will find this criterion in the next two theorems, extracted again from Ref. [28].

Theorem 2.—Let $V(a)$ be a continuous real-valued function on $(0,\infty)$ and suppose that there exists a positive differentiable function $M(a)$, so that

(i) $V(a) \geq -M(a)$,
(ii) $\int_1^\infty \sqrt{M(a)}da = \infty$,
(iii) $M(a)/(M(a))^{3/2}$ is bounded near ∞.

Then $V(a)$ is in the limit point case at ∞.

Theorem 3.—Let $V(a)$ be continuous and positive near $a = 0$. If $V(a) \geq \frac{3}{4a^2}$ near zero then $-d^2/da^2 + V(a)$ is in the limit point case at zero. If for some $\epsilon > 0$, $V(a) \leq (\frac{3}{4} - \epsilon)a^{-2}$ near zero, then $-d^2/da^2 + V(a)$ is in the limit circle case.

From now on, we will consider $g_s < 0$. In the end of this section, we will return to the case $g_s > 0$. Let us first use Theorem 2 to show that the Hamiltonian operator in Eq. (47) is in the limit point case at infinity. To verify this fact, note that the potential $V(a)$ has a minimum $V_{\min} = 2m_\lambda[\sqrt{-2g_s}m_\lambda^{1/2}\omega_\lambda - g_r]$ at $a = (\frac{-2g_s}{m_\lambda})^{1/4}\omega_\lambda^{-1/2}$. If $V_{\min} \geq 0$, we choose $M(a) = 1$ and all the requirements of Theorem 2 are fulfilled. If $V_{\min} \leq 0$, we take $M(a) = |V_{\min}|$. In any case, we conclude that $\hat{H}$ is in the limit point case at infinity.

Note now that the potential $V(a)$ has the form $V(a) \sim -2m_\lambda g_s/a^2$ near $a = 0$. Therefore, by Theorem 3, if $-2m_\lambda g_s \geq 3/4$ then $\hat{H}$ is in the limit point case at zero; otherwise, it is in the limit circle case. We have established a range of parameters in which the operator $\hat{H}$ is essentially self-adjoint, i.e., if

$$-m_\lambda g_s \geq 3/8, \tag{51}$$

then the evolution of the wave function representing the universe is uniquely determined by the initial wave packet and no boundary condition at $a = 0$ is necessary. Otherwise, we need to impose a boundary condition at this point. For simplicity we did not consider the case $\Lambda \neq 0$, but the previous analysis still works in this case.

It turns out that Eq. (47) can be solved exactly. By introducing the new variable $x = \sqrt{m_\lambda \omega_\lambda} a$ and a parameter [32]

$$\alpha = \frac{1}{2}\sqrt{1 - 8m_\lambda g_s}, \tag{52}$$

Eq. (47) becomes

$$-\frac{d^2}{dx^2}\psi(x) + \left[x^2 - \frac{2}{\omega_\lambda}(gr + E) + \frac{4\alpha^2 - 1}{4x^2}\right]\psi(x) = 0. \tag{53}$$

By introducing the new function $y(\eta)$ given by

$$\psi(x) = e^{-\frac{x^2}{2}} x^{\alpha + 1/2} y(x^2), \tag{54}$$

it is easy to see that $y(\eta)$ satisfies the associated Laguerre equation

$$\eta y''(\eta) + (1 + \alpha - \eta) y'(\eta) + \lambda_E y(\eta) = 0, \tag{55}$$

where

$$\lambda_E = \left[\frac{(E + g_r)}{2\omega_\lambda} - \frac{(1 + \alpha)}{2}\right]. \tag{56}$$

This equation is known to be Hermitian (formally self-adjoint) with the inner product

$$\langle f, g \rangle_L = \int_0^\infty e^{-\eta} \eta^\alpha \overline{f(\eta)} g(\eta) d\eta. \tag{57}$$

The general solution of Eq. (55) is given by [33]

$$y(\eta) = A_E M(-\lambda_E, 1 + \alpha, \eta) + B_E U(-\lambda_E, 1 + \alpha, \eta), \tag{58}$$

where M and U are the confluent hypergeometric functions of the first and second kinds, respectively. For $\lambda_E = n = 0, 1, 2, \ldots,$ both M and U are polynomials of degree n, proportional to the associated Laguerre polynomial $L_n^\alpha(\eta)$. The other linearly independent solution is not square-integrable near $a = 0$, so it must be excluded from the present analysis. If $\lambda_E \notin \mathbb{N} \cup \{0\}$, we have the following asymptotic behavior for M and U, as $\eta \to \infty$:

$$M(-\lambda_E, 1 + \alpha, \eta) \sim \frac{\Gamma(1 + \alpha)}{\Gamma(-\lambda_E)} e^\eta \eta^{-1-\lambda_E-\alpha},$$
$$U(-\lambda_E, 1 + \alpha, \eta) \sim \eta^{\lambda_E}. \tag{59}$$

Therefore, M is not square-integrable near infinity, whereas U is. Thus, M is not an acceptable solution in this case. As $\eta \to 0$, the asymptotic behavior of U is given by

$$U(-\lambda_E, 1 + \alpha, \eta) \sim \eta^{-\alpha}\Gamma(\alpha)/\Gamma(-\lambda_E), \tag{60}$$

and, hence, U is square-integrable near $a = 0$ only if $\alpha < 1$. For $\alpha \geq 1$, we do not have an acceptable solution, except in the case $\lambda_E = n = 0, 1, 2, \ldots$. Therefore, for $\alpha \geq 1$ (which corresponds to $-m_\lambda g_s \geq 3/8$), we automatically quantize the energy levels of the universe, which are given by

$$E_n = (2n + 1 + \alpha)\omega_\lambda - g_r. \tag{61}$$

The corresponding normalized eigenstates are given by

$$\Psi_n(a,t) = (4m_\lambda\omega_\lambda)^{1/4}\left[\frac{\Gamma(n+1)}{\Gamma(\alpha+n+1)}\right]^{1/2}(m_\lambda\omega_\lambda a^2)^{\frac{2\alpha+1}{4}} \times \exp\left(-\frac{m_\lambda\omega_\lambda}{2}a^2\right)L_n^\alpha(m_\lambda\omega_\lambda a^2)e^{-iE_n t}, \tag{62}$$

and a general solution $\Psi(a, t)$, depending on the initial wave packet $\Psi(a, 0)$, is then given by

$$\Psi(a, t) = \sum_{n=0}^\infty c_n \Psi_n(a, t), \tag{63}$$

with

$$c_n = \int_0^\infty \Psi(a, 0)\Psi_n^*(a, 0) da. \tag{64}$$

For $1/2 \leq \alpha < 1$, Eq. (60) shows that U is square-integrable at $a = 0$. We then need a boundary condition at $a = 0$ in order to have a well posed Sturm-Liouville problem. They are found in Ref. [34] and are given by

$$\Gamma_1 y = \theta \Gamma_0 y, \qquad \theta \in \mathcal{R}, \tag{65}$$

where

$$\Gamma_0 y = \lim_{x\to 0} x^{\alpha+1} y'(x), \quad \Gamma_1 y = \lim_{x\to 0}\left[y(x) + \frac{x}{\alpha} y'(x)\right]. \tag{66}$$

If $\theta = \infty$, then $\lim_{x\to 0} x^{\alpha+1} y'(x) = 0$ and we find that [35] $\lambda_E = n = 0, 1, 2, \ldots,$ and the corresponding associated Laguerre polynomials. For other values of θ, the quantized energy levels are not so simple. In all cases, the wave function will satisfy the DeWitt condition,

$$\Psi(0, t) = 0, \tag{67}$$

but we stress the fact that this is not the condition which turns the Wheeler-DeWitt equation into a self-adjoint form.

It is worth analyzing the case $\lambda \to 1$, $g_r \to 0$, and $\alpha \to 1/2$, where we expect to recover the usual quantum cosmology. In this limit, Eq. (62) becomes

$$\Psi_n(a,t) = \left(\frac{\sqrt{48}}{\sqrt{\pi}2^{2n+1}(2n+1)!}\right)^{1/2} H_{2n+1}(\sqrt{12}a)e^{-6a^2}e^{-iE_n t}, \tag{68}$$

with

$$E_n = 2n + 3/2. \tag{69}$$

These same eigenstates have already been found in Ref. [19] in the context of ordinary quantum cosmology. They satisfy the Dirichlet boundary condition $\Psi(0, t) = 0$. The Neumann boundary condition is satisfied when $\alpha \to -1/2$. We do not consider this case here, but it is trivial to generalize our results to $-1 < \alpha < 1/2$ (see Ref. [34]). Therefore, the HL quantum cosmology tends naturally to the usual quantum cosmology in the appropriate limit.

Having studied the self-adjointness of the evolution equation of the universe, let us now focus on the evolution of the expectation value of the scale factor given a solution representing the state of the universe. Obviously, if we calculate the expectation value of the scale factor in any of these eigenstates it will be constant. But the universe evolves in such a way that we must consider wave packets representing the state of the universe. In order to find exact solutions, we choose an initial wave packet of the form

$$\Psi(a, 0) = \left[\frac{2^{\nu+5/2}\sigma^{\nu+3/2}}{\Gamma(\nu + 3/2)}\right]^{1/2} a^{\nu+1} e^{-\sigma a^2}, \qquad (70)$$

where $g_s = -\nu(\nu + 1)/(2m_\lambda)$. Note that $g_s < 0$ in this case, so that the potential $V(a)$ is repulsive, preventing the formation of a classical singularity. The propagator for Eq. (47) is given by [36]

$$G(a, a'; t; \nu) = \frac{m_\lambda \omega_\lambda \sqrt{aa'}}{\sin(\omega_\lambda t)} e^{ig_r t} i^{-(\nu+3/2)} \times \exp\left[\frac{i m_\lambda \omega_\lambda}{2} \cot(\omega_\lambda t)(a^2 + a'^2)\right] \times J_{\nu+1/2}\left(\frac{m_\lambda \omega_\lambda a a'}{\sin(\omega_\lambda t)}\right), \qquad (71)$$

and through the equation

$$\Psi(a, t) = \int_0^\infty G(a, a'; t; \nu)\Psi(a', 0) da', \qquad (72)$$

we find, after some tedious calculation,

$$\Psi(a, t) = \left[\frac{2^{\nu+5/2}\sigma^{\nu+3/2}}{\Gamma(\nu + 3/2)}\right]^{1/2} \left(\frac{m_\lambda \omega_\lambda}{i \sin(\omega_\lambda t)}\right)^{\nu+3/2} \times \frac{a^{\nu+1} e^{ig_r t}}{[2\sigma - i m_\lambda \omega_\lambda \cot(\omega_\lambda t)]^{\nu+3/2}} \times \exp\left(\frac{-m_\lambda^2 \omega_\lambda^2 \sigma a^2}{4\sigma^2 \sin^2(\omega_\lambda t) + m_\lambda^2 \omega_\lambda^2 \cos^2(\omega_\lambda t)}\right) \times \exp\left[\frac{i m_\lambda \omega_\lambda \sin(\omega_\lambda t)\cos(\omega_\lambda t) a^2}{2(4\sigma^2 \sin^2(\omega_\lambda t) + m_\lambda^2 \omega_\lambda^2 \cos^2(\omega_\lambda t))} \times (4\sigma^2 - m_\lambda^2 \omega_\lambda^2)\right]. \qquad (73)$$

The expectation value of the scale factor is given by

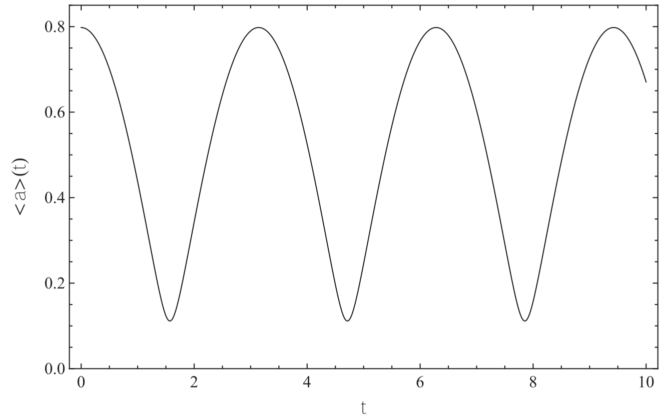

FIG. 1. The evolution of the scale factor in the case of an attractive potential. Twenty terms in the expansion Eq. (63) were used in this numerical approximation.

$$\langle a\rangle(t) = \frac{\Gamma(\nu + 2)}{\sqrt{2\sigma}\Gamma(\nu + 3/2)} \frac{1}{m_\lambda \omega_\lambda} \times \sqrt{4\sigma^2 \sin^2(\omega_\lambda t) + m_\lambda^2 \omega_\lambda^2 \cos^2(\omega_\lambda t)} = \frac{\langle a\rangle(0)}{m_\lambda \omega_\lambda} \sqrt{4\sigma^2 \sin^2(\omega_\lambda t) + m_\lambda^2 \omega_\lambda^2 \cos^2(\omega_\lambda t)}. \qquad (74)$$

We stress the nonsingular character of the above equation, since $\langle a\rangle(t) \neq 0$ for all times. As in the usual quantum cosmology [19], the singularity is not present in the quantum model. Note also the similarity with the results found in Ref. [19]. The only difference here is that the parameter λ changes the frequency of oscillation of the scale factor. The behavior of this quantum universe in HL theory is not very different from the usual quantum cosmology.

We can also study the case $g_s > 0$, when the potential $V(a)$ is attractive, which does not prevent the formation of a classical singularity. In order to obtain exact solutions we must restrict $2m_\lambda g_s \leq 1/8$ so that $\alpha \geq 0$. We do not have a propagator in this case, but we can use Eq. (63) to numerically find the evolution of the scale factor. This is done in Fig. 1, where we have chosen an initial wave packet of the form

$$\Psi(a, 0) = 2\left(\frac{8}{\pi}\right)^{1/4} a e^{-a^2}. \qquad (75)$$

The parameters characterizing HL gravity are $\lambda = 1$, $gr = 0$, and $\alpha = 1/4$. Note that $\langle a\rangle(t) \neq 0 \forall\ t$. The singularity has been excluded.

VII. CONCLUDING REMARKS

We have seen that in the HL theory of gravity, it is possible to not only exclude the initial big bang singularity, but also to uniquely determine the evolution of the wave function of the universe given an initial wave packet. An equivalent statement is that no boundary condition at $a = 0$ is necessary in a quantum cosmology in the context of HL gravity. In general, theories of gravity do not tell us which boundary condition we must choose, so it is a remarkable fact that one of these theories excludes this ambiguity. Moreover, in HL quantum cosmology the evolution of the expectation value of the scale factor resembles the evolution found in usual quantum cosmology, the only difference being the frequency of oscillation of the bouncing universe. It is interesting to notice that the quantum regime of the HL theory of gravity can also provide a viable framework for the description of the ''asymptotic darkness'' of the visible universe [37]. Our early universe results are in a certain sense complementary to the asymptotic regime described in Ref. [37]. It is certainly worthwhile to further explore the connections between the two approaches.

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