Effective gravity formulation that avoids singularities in quantum FRW cosmologies

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Assuming that time exists, a new, effective formulation of gravity is introduced, which lies in between the Wheeler-DeWitt approach and ordinary QFT. Remarkably, the Penrose-Hawking singularity of usual Friedman-Robertson-Walker cosmologies is naturally avoided there. The theory is made explicit via specific examples, and compared with loop quantum cosmology. It is argued that it is the regularization of the classical Hamiltonian performed in this last theory what avoid the singularity, rather than quantum effects as in our case.

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I. INTRODUCTION

In accordance with the celebrated Penrose-Hawking singularity theorem, Friedman-Robertson-Walker (FRW) cosmologies give rise to a singularity when the strong energy condition holds, $\rho + 3p > 0$, $\rho$ being energy density and $p$ pressure [1]. A simple way to avoid this singularity is introducing a scalar field that breaks the strong energy condition [2-4]. Another possibility is to consider quantum effects due to vacuum polarization, as the one due to a massless scalar field conformally coupled with gravity [5, 6, 7]. Remarkably, there is a very natural and fundamental alternative: to depart from the Wheeler-DeWitt equation, $\dot{H}\Phi = 0$ [8, 9], with $\dot{H}$ the quantum Hamiltonian, by assuming that time has an absolute meaning. The question of a possible singularity is then addressed in terms of a Schrödinger equation with additional conditions, what specifically defines our theory:

$$i\hbar \partial_t \Phi(t) = \hat{H}\Phi(t), \quad \Phi(t^*) = \Psi, \quad \langle \hat{H}\rangle_\Psi = 0, \quad ||\Psi|| = 1. \quad (1)$$

We thus plainly assume the choice of a time direction to have a physical solution, what goes against common lore. In this sense our approach is absolutely original, revolutionary and, as we will prove, clarifying and predictive.

Some basic technical details on what will be demonstrated below. The quantum Hamiltonian $\hat{H}$, obtained with the usual rules of quantum mechanics, is generically symmetric but not self-adjoint. By von Neumann’s theorem [10, 11], it can be extended to a self-adjoint operator (sometimes in infinitely many ways). Stone’s theorem then applies, leading to a solution valid at all time $t$ and, consequently, we can compute the average of the quantum operator $\hat{a}$ corresponding to the classical scale factor $a$. That is, we compute the following effective scale factor $a_{eff}(t) = \langle \Phi(t) | \hat{a} | \Phi(t) \rangle$, where $\Phi(t)$ is the solution of the effective Schrödinger equation above. It is not difficult to see that if $\Phi(t)$ belongs to the domain of the operator $\hat{a}$ at any time, then the effective scale factor is always strictly positive, and we can conclude that the singularity is avoided. Physically, the self-adjoint extension of the Hamiltonian operators that appears in FRW cosmologies can be understood assuming that there is an infinitely barrier potential at the point $a = 0$, then when the effective factor scales approaches to zero, at some finite time, it bounces and grows.

However to compute averages one usually works in Heisenberg’s picture, so $\hat{A} = \frac{1}{i}[\hat{H}, \hat{A}]$, for any operator involved in the calculation. But, using this formula one turns out to obtain, at some finite time, a negative value for the average of the scale factor operator. Such a contradictory result can be explained by the fact that, at some finite time, the commutator between the Hamiltonian and the operator $\hat{A}$ is not well defined, what invalidates the final result (physically one can explain this taking into account that in Heisenberg picture the boundary conditions do not appear, i.e., the barrier potential are not introduced and then the effective factor scale has the freedom to take all the values in $\mathbb{R}$). That is, the average of the scale factor is positive, but we do not have any method to obtain an analytic information about its behavior, because the Heisenberg picture fails to work, and it also turns out to be impossible to obtain an explicit solution of the effective Schrödinger equation. To this end loop quantum cosmology (LQC) will be invoked [12-14]. In what follows, we present a simple demonstration of the above approach and will explicitly see how this theory avoids the singularity. It will be also shown that it is the regularization of the classical Hamiltonian [14, 15, 16] what avoid the singularity, rather than quantum effects.

In the first of the three Appendix in the paper we present a brief mathematical review about the theory of self-adjoint extensions of symmetric operators based on Von Neumann’s theorem. In the second one, we apply the effective formulation to the case of a barotropic fluid where on can see clearly the physical meaning of the self-adjoint extension of a symmetric operator. As specific examples, the dust and radiation cases are treated in detail, showing that the self-adjoint extensions of the respective
Hamiltonian operators can be understood assuming that there is an infinitely barrier of potential at \( a = 0 \). Finally in the last one, we show (resp. review) how to derive the standard quantum fields theory in curved space-time from the effective formulation (resp. the Wheeler-DeWitt equation). We also obtain, from the effective formulation, the semi-classical Einstein equation, that is, the back-reaction equation.

II. THE PROBLEM

In this Section we consider an homogeneous and isotropic gravitational field minimally coupled to an homogeneous scalar field, which Lagrangian is given by \([4]\)

\[
L(t) = \frac{3c^2}{8\pi G} (c^2 \ddot{a} - \dot{a}^2) a + \frac{1}{2} \dot{\phi}^2 a^3 - V(\phi) a^3, \tag{2}
\]

where \( G \) is Newton’s constant and \( k \) the three-dimensional curvature. We are interested in the case \( k = 0 \) and \( V \equiv 0 \), previously studied in \([17,18]\) within the framework of LQC. This interest comes from the fact that in the chaotic inflationary model with \( V \gg m^2 \dot{\phi}^2 \), at very early times before the inflationary period, one has \( \phi \gg V \) (see for details \([19]\)). Then the potential can be neglected and one has \( \rho \equiv p \). Consequently this model give rise to a singularity at very early times, that we want to avoid using the effective formulation described in the Introduction.

Defining the angle variable \( \psi = \sqrt{3c^2/4\pi G} \psi \), the Lagrangian becomes \((l_p \text{ denotes the Planck length})\)

\[
L = -\frac{\gamma^2}{2}(\dot{a}^2 a - \dot{\psi}^2 a^3), \quad \text{with} \quad \gamma^2 = \frac{3c^2}{4\pi G} = \frac{3\hbar}{4\pi cl_p^2}. \tag{3}
\]

Using the conjugate momenta, \( p_a = -\gamma^2 \dot{a} a \) and \( p_\psi = \gamma^2 \dot{\psi} a^3 \), we can write the Hamiltonian as

\[
H = \frac{1}{2\gamma^2 a^3} [-(ap_a)^2 + p_\psi^2]. \tag{4}
\]

The classical dynamic equations are

\[
\dot{a} = -\frac{1}{\gamma^2 a^2} ap_a, \quad (ap_a) = 3H, \quad \dot{\psi} = \frac{1}{\gamma^2 a^3} p_\psi, \quad \dot{p}_\psi = 0, \tag{5}
\]

together with the constraint \( H = 0 \), that is \((ap_a)^2 = p_\psi^2\). Integrating \(5\) we obtain the following solution

\[
0 > a(t) p_a(t) = p_a^*, \quad p_{\psi \pm}(t) = p_{\psi \pm}^* = \pm p_a^*, \tag{6}
\]

\[
a(t) = a^* \left[ 1 - \frac{3p_a^*(t - t^*)}{\gamma^2 (a^*)^3} \right]^{1/3}, \quad \psi_{\pm}(t) = \mp \ln \frac{a(t)}{a^*} + \psi^*. \]

Note that the solution \((a(t), \psi_{\pm}(t))\) is defined in the interval \((t_s, +\infty)\), where \( t_s = t^* + (\gamma^2/3p_a^*)(a^*)^3 \). At this time we have \( a(t_s) = 0 \), and \( \psi_{\pm}(t_s) = \pm \infty \), that is, the dynamics is singular at \( t = t_s \). Note that we can write \( a(t) = a^* \left[ 1 - (t - t^*)/(t_s - t^*) \right]^{1/3} \). Finally, we see that from Eqs. \(5\) we have \( d\ln a/d\psi_{\pm} = \mp 1 \), and conclude:

\[
a = a^* e^{\mp(\psi_{\pm} - \psi^*)}. \tag{7}
\]

A. Quantum dynamics

We now use the quantization rule:

\[
g^{AB} p_A p_B \longrightarrow -\hbar^2 \nabla_A \nabla^A = -\frac{\hbar^2}{\sqrt{|g|}} \partial_A (\sqrt{|g|} g^{AB} \partial_B), \tag{8}
\]

and obtain the quantum Hamiltonian

\[
\hat{H} \equiv \frac{\hbar^2}{2\gamma^2 a^3} (a \partial_a a \partial_a - \partial_{\psi^2}). \tag{9}
\]
Introducing the operators \( \widehat{a}^\dagger a \equiv -\hbar a^{-1/2}\partial_\alpha a^{3/2} \); \( \hat{p}_\psi \equiv -i\hbar\partial_\psi \), we can write \( \hat{H} \equiv \frac{1}{2\gamma}a^{-3/2}\hat{p}_\psi^2 - (\widehat{a}^\dagger a)^2 a^{-3/2} \). The dynamical equations in the Heisenberg picture are

\[
\frac{d\hat{a}}{dt} = -\frac{1}{\gamma^2 a^2}((\widehat{a}^\dagger a + i\hbar), \quad \frac{d(\widehat{a}^\dagger a)}{dt} = 3\hat{H},
\]

\[
\frac{d\hat{\psi}}{dt} = \frac{1}{\gamma^2 a^2}\hat{p}_\psi, \quad \frac{d\hat{p}_\psi}{dt} = 0,
\]

with \( \langle \Phi \vert \Psi \rangle \equiv \int_0^\infty d\psi\psi^\dagger\Phi^*(a,\psi)a^2\psi(a,\psi) \) as inner product and operator average \( \langle \hat{A} \vert \Psi \rangle \equiv \langle \Psi \vert \hat{A} \Psi \rangle \), \( ||\Psi|| = 1 \).

**Example 1.** Consider the wave-function \( \langle p^*_t \vert \rangle \equiv \langle p^*_\psi \vert \rangle : \Phi(a,\psi) \equiv \frac{1}{\gamma}(\ln(\alpha/a))^2 e^{-\frac{(\psi - a^2)^2}{2\alpha}} e^{\frac{\pi}{\hbar}\left(\ln(\alpha/a)p^*_\psi + \psi p^*_\psi \right)} \). Then:

\( \langle \hat{a} \rangle \psi = ae^{\gamma/4} \equiv a^*, \langle \hat{\psi} \rangle \psi = \psi^*, \langle \widehat{a}^\dagger a \rangle \psi = p^*_\alpha, \langle \hat{p}_\psi \rangle \psi = p^*\psi, \) and \( \langle \hat{H} \rangle \psi = 0 \).

**B. The Wheeler-DeWitt equation**

Compare at this point with the Wheeler-DeWitt equation paradigm (WDW) \( \hat{H} \Phi = 0 \rightarrow (a\partial_\alpha a - \partial^2_\psi)\Phi = 0 \),

with general solution \( (a \text{ is a length constant}) \)

\( \Phi(a,\psi) = f_+(\ln(a/\alpha) + \psi) + f_-(\ln(a/\alpha) - \psi) \).

The quantum version of Eq. (7) is \( \Phi_+(a,\psi) = f_+(\ln(\alpha/a)^* + \psi^*), \Phi_-(a,\psi) = f_-(\ln(\alpha/a)^* - \psi + \psi^*), \) with \( f_\pm \) a function picked around 0, as for instance \( f_+(z) = e^{-z^2/\sigma}. \) From this result we see that the wave is always picked around the classical solution, but we cannot conclude that its dynamical behavior is singular since here time does not appear.

In order to understand the dynamics, we postulate the effective equation (11). Note that \( \langle \hat{H} \rangle \psi = 0 \) implies \( \langle \hat{H} \rangle \dot{\phi}(t) = 0 \), and \( ||\Psi|| = 1 \) implies \( ||\Phi(t)|| = 1 \), \( \forall \dot{t} \in \mathbb{R} \). Then, if the solution of the problem exists for all \( \dot{t} \), it is easy to prove that the effective scalar factor, \( a_{eff}(t) \equiv \langle \hat{a} \rangle \dot{\phi}(t) \), never vanishes. In fact, the condition \( ||\Phi(t)|| = 1 \), \( \dot{t} = \infty \), \( \Phi(t, a, \psi)^2 = 1 \) and thus we have: \( a_{eff}(t) = \langle \hat{a} \rangle \dot{\phi}(t) = \int_0^\infty d\psi \psi^2 \Phi(t, a, \psi)^2 = 0 \).

To do the calculation, we consider the quantity \( \langle \hat{a}^3 \rangle \Phi(t) \). We have \( \frac{d}{dt} \langle \hat{a}^3 \rangle \Phi(t) = \frac{3}{2} \langle \hat{a} \hat{a}^2 \rangle \Phi(t) = -\frac{3}{2} \langle \hat{a}^\dagger a \rangle \Phi(t) = \frac{3}{2} \langle \hat{a}^3 \rangle \Phi(t) = 0 \) due to the remark above. Consequently, we obtain

\( \langle \hat{a}^3 \rangle \Phi(t) = \langle \hat{a}^3 \rangle \Phi(0) \).

For the function of Example 1, we get

\( \langle \hat{a}^3 \rangle \Phi(t) = a^3 e^{3\sigma/4} - \frac{3}{2} a^3 \hat{p}_\psi(t - t^*), \)

and this contradicts the fact that \( \langle \hat{a}^3 \rangle \Phi(t) \geq 0, \forall \dot{t} \in \mathbb{R} \). However, since the operator \( \hat{H} \) is symmetric and real, using von Neumann’s theorem \( \text{[10, 11]} \) it can be extended to a self-adjoint one, and then the solution of the problem (11) exists here for any \( t \) (Stone’s theorem). From this result, we conclude that there is a value of \( t \) for which some of the commutators \( [\hat{H}, \hat{a}^3] \) and/or \( [\hat{H}, \hat{a}^\dagger a] \) do not exist; thus the final result (14) is incorrect. The drawback of this method is the lack of an analytic procedure to calculate the average since, in general, there is no explicit formula that gives information on the regular behavior of the average of the scale factor operator. Fortunately, a useful way exists to directly analyze the singularity, namely loop quantum cosmology (LQC). Before using it in our problem, we consider another example where the above contradictions can be easily depicted.

**Example 2.** Consider now the problem

\( i\partial_t \Phi = -i\hbar c\partial_\alpha \Phi \equiv c\hat{p_\phi} \Phi, \quad \forall x \in [0, 2\pi], \quad \Phi(0) = \Psi, \)

being \( \hat{p} \) self-adjoint in the domain \( \text{[11]} \): \( D_\rho = \{ \Phi \text{ absolutely continuous in } [0, 2\pi], \partial_x \hat{\Phi} \in L^2[0, 2\pi], \}

\( \Psi(0) = \Psi(2\pi) \}. \) Let \( \Phi(t) \) be the solution of our effective formulation (15). We want to calculate \( \langle \hat{\dot{x}} \rangle \Phi(t) = \int_0^{2\pi} x|\Phi(t, x)|^2 dx. \)

Using \( [\hat{p}, \hat{x}] = -i\hbar \), we get \( \langle \hat{\dot{x}} \rangle \Phi(t) = c \), i.e., \( \langle \hat{\dot{x}} \rangle \Phi(t) = \langle \hat{x} \rangle \Phi + ct \) which is **not** positive \( \forall t \). What actually happens is that, for
Fourier analysis provides the following solution of the Schrödinger equation for small values of $\hbar$:

$$\Psi(x) = \sqrt{\frac{3}{2\pi^2}} \left\{ \begin{array}{ll} x, & \text{for } x \in [0, \pi], \\
2\pi - x, & \text{for } x \in [\pi, 2\pi]. \end{array} \right.$$  \hfill (16)

Fourier analysis provides the following solution of the Schrödinger equation

$$\Phi(t, x) = \sqrt{\frac{3}{2\pi^2}} \left\{ \begin{array}{ll} \frac{\pi}{2} - \frac{4}{\pi} \sum_{n \in \mathbb{Z}} \frac{1}{(2n + 1)^2} \cos [(2n + 1)(x - ct)] \end{array} \right. .$$

Then, at $t = 0$ we have $x\Phi(0, x) \in D_ρ$ but if we choose $t = \pi/c$ we obtain $x\Phi(\pi/c, x) |_{t=0} = 0$, and $x\Phi(\pi/c, x) |_{t=2\pi} = \sqrt{6}\pi/c$, what means effectively that $x\Phi(\pi/c, x) \not\in D_ρ$. However, note that $(\dot{x})_\Phi(t)$ exists for all $t \in \mathbb{R}$, its value being:

$$0 < \langle \dot{x} \Phi(t) \rangle = \int_{0}^{2\pi} 3x \sqrt{\frac{3}{2\pi^2}} \left\{ \begin{array}{ll} \frac{\pi}{2} - \frac{4}{\pi} \sum_{n \in \mathbb{Z}} \frac{1}{(2n + 1)^2} \cos [(2n + 1)(x - ct)] \end{array} \right\}^2 dx < 2\pi.$$

III. LOOP QUANTUM COSMOLOGY TO RESCUE

We shall now involve (a simplified version of) LQC (for a rigorous formulation see [13, 16]), with different variables and a different quantum space of states, adapted to make contact with our theory above.

Consider the variables $p \equiv a^2$ and $x \equiv a$. Their Poisson bracket is $\{x, p\} = \frac{\sin x}{x^2} = \frac{2}{\pi}$. We also consider the holonomies $h_j(n) \equiv e^{-i\frac{\pi}{\hbar} \sigma_j} = \cos \left( \frac{\pi n}{\hbar} \right) - i\sigma_j \sin \left( \frac{\pi n}{\hbar} \right)$ [21], where $\sigma_j$ are the Pauli matrices and $i$ is the Barbero-Immirzi parameter. We easily obtain Ashtekar-Barbero’s formula [21]:

$$a^{-1} = -\frac{i\hbar}{4\pi l_p^2} \text{Tr} \left[ \sum_{j=1}^{3} \sigma_j h_j(1) \{h_j^{-1}(1), a\} \right].$$

To get the gravitational part of the Hamiltonian, we cannot directly use this one: $H_{\text{grav}} = -\frac{\gamma^2 c^2 a^2}{2\epsilon^2} \sqrt{\epsilon}$, which leads to singular classical dynamics. We may use the general formulae of loop quantum gravity (LQG) to obtain the regularized Hamiltonian [9, 16, 18]:

$$H_{\text{grav,}\epsilon} = -\frac{\hbar^2 c}{32\pi^2 l_p^4} \sum_{i,j,k} \epsilon^{ijk} \text{Tr} \left[ h_i(1) h_j(1) h_k^{-1}(1) h_i^{-1}(1) h_k(1) \{h_k^{-1}(1), a^3\} \right] = -\frac{\gamma^2 c^2}{2\epsilon^2} a \sin^2 \frac{tx}{c},$$

which is bounded when the extrinsic curvature $x/2$ (a half of the velocity of the scalar factor) diverges, and approaches $H_{\text{grav}}$ for small values of $x$. Then, taking this regularized Hamiltonian as the gravitational part of the full one, this last is given by [20, 21]:

$$H_i \equiv -\frac{\gamma^2 c^2}{2\epsilon^2} a^2 \sin^2 \frac{tx}{c} + \frac{1}{2\epsilon^2} a^{-3} p_\psi^2 ,$$

and the dynamical equations are

$$\dot{a} = \{a, H_i\} = \frac{c}{2\epsilon^2} \sin \frac{2tx}{c}, \quad \dot{x} = \{x, H_i\} = -\frac{2}{\gamma^2} a^2 p_\psi^2.$$  \hfill (19)

Imposing the Hamiltonian constraint $H_i = 0$, we obtain

$$\dot{a}^2 = \frac{p_\psi^4}{\gamma^4 a^4} \left( 1 - \frac{p_\psi^2 c^2}{\gamma^4 a^4} \right).$$  \hfill (20)

and since $p_\psi \equiv p_\psi^*$ is constant, we get the following bounce, $\dot{a} = 0$ when $a = \frac{1}{\gamma} \sqrt{\frac{p_\psi^2 c^2}{\gamma^4}} = 2l_p \sqrt{\frac{\pi p_\psi^4}{3\hbar}}$. Consequently, there is no singularity because the range of $a(t)$ is $\left[ 2l_p \sqrt{\frac{\pi p_\psi^4}{3\hbar}}, +\infty \right]$, $\forall t \in \mathbb{R}$. In fact, at earlier times the scalar factor is very big, then it
decreases, and when it arrives at the turning value it increases forever. Moreover, this solution yields a period of inflation \[20\], namely, from the Friedmann Eq. \(20\): \(\dot{a} > 0\), for \(a \in \left(2l_p \sqrt{\frac{\pi p_{\psi}^2}{3\hbar}}, 2l_p \sqrt{\frac{\sqrt{2}\pi p_{\psi}^2}{3\hbar}}\right)\). Finally, note that when \(a \gg l_p\), Eq. \(20\) coincides with \(5\).

A different way to understand these features is to write Eq. \(20\) as \((\dot{a}/a)^2 = \frac{2\rho_{\text{eff}}}{\gamma^2}\), where we have introduced the effective energy density \(\rho_{\text{eff}} = \frac{\rho^2}{p_{\psi}^2} \left(1 - \frac{p_{\psi}^2}{\gamma^2 c^2}\right)\). Taking the derivative, \(\dot{\rho}_{\text{eff}} = -3 \left(\frac{\dot{a}}{a}\right) (\rho_{\text{eff}} + p_{\text{eff}})\), where the effective pressure is \(p_{\text{eff}} = \frac{p_{\psi}^2}{2\gamma^2}\left(1 - \frac{7p_{\psi}^2}{3\gamma^2 c^2}\right)\). But then it is easy to see that the strong energy condition \(\rho_{\text{eff}} + 3p_{\text{eff}} > 0\) is broken, when the scale factor lies in the interval \(\left(2l_p \sqrt{\frac{\pi p_{\psi}^2}{3\hbar}}, 2l_p \sqrt{\frac{\sqrt{2}\pi p_{\psi}^2}{3\hbar}}\right)\), consequently, the singularity is avoided. Moreover, for \(a \in \left(2l_p \sqrt{\frac{\pi p_{\psi}^2}{3\hbar}}, 2l_p \sqrt{\frac{\sqrt{2}\pi p_{\psi}^2}{3\hbar}}\right)\), there is a period of super-inflation; that is, in this interval, one has \(\frac{\rho_{\text{eff}}}{p_{\text{eff}}} < -1\).

The following remark is in order. Similar results are obtained in the case \(k = 1\) and \(V \equiv 0\). Now the classical Hamiltonian is given by

\[
H = \frac{1}{2\gamma^2 a^3} \left(-\left(ap_{\psi}\right)^2 + p_{\psi}^2 - \gamma^4 c^2 a^4\right),
\]

and the regularized one, is

\[
\tilde{H}_r = -\frac{\gamma^2 c^2}{2l^2} a \left(\sin^2 \left(\frac{\ell x}{c}\right) - c^2\right) + \frac{1}{2\gamma^2} a^{-3} p_{\psi}^2.
\]

Then, using the Hamiltonian constraint \(\tilde{H}_r = 0\), is easy to obtain the Friedmann equation

\[
\dot{a}^2 = \left(\frac{\tilde{p}_{\psi}^2}{\gamma^4 a^4} - c^2\right) \left(1 + \ell^2 - \frac{\tilde{p}_{\psi}^2 \ell^2}{\gamma^4 a^4 c^2}\right),
\]

and since, \(p_{\psi} = p_{\psi}^0\) is constant and \(\dot{a}^2 \geq 0\), we can deduce that \(a \in \left[2l_p \sqrt{\frac{\pi p_{\psi}^2}{3\hbar}}, 2l_p \sqrt{\frac{\sqrt{2}\pi p_{\psi}^2}{3\hbar}}\right]\), and clearly the singularity is avoided. In this case, we have an oscillating universe.

Another equivalent way to do this, is to use the variable \(\tilde{x} \equiv \dot{a} + c\), then following \(23, 24\) we obtain the regularized hamiltonian

\[
\tilde{H}_r = -\frac{\gamma^2 c^2}{2l^2} a \left(\sin^2 \left(\frac{\ell (\tilde{x} - c)}{c}\right) - \sin^2 (\ell) + 2\ell^2\right) + \frac{1}{2\gamma^2} a^{-3} p_{\psi}^2.
\]

It is clear, that from this last regularized hamiltonian the scale factor has the same behavior that described in equation \(23\).

### A. Quantization

To quantize we perform the usual change \(\{A, B\} \rightarrow -\frac{i}{\hbar} [\hat{A}, \hat{B}]\). Note that the system is \(\frac{4\pi c}{\hbar}\)-periodic with respect to the variable \(x\), thus we consider the space of \(\frac{4\pi c}{\hbar}\)-periodic functions and introduce the inner-product \(\langle \Psi, \Phi \rangle = \int_{\mathbb{R}} dx \Psi^*(x) \phi(x) \phi(x)\). Completion of this space with respect to this product is the space of square-integrable functions in \([-\frac{4\pi c}{\hbar}, \frac{4\pi c}{\hbar}]\). Note that, rigorously, the definition of the Hilbert space is more complicated: \(L^2(\mathbb{R}_{Bohr}, d\mu_{Bohr})\) where \(\mathbb{R}_{Bohr}\) is the compactification of \(\mathbb{R}\) and \(\mu_{Bohr}\) the Haar measure on it \(18\). However, for our purposes the Hilbert space \(L^2([-\frac{4\pi c}{\hbar}, \frac{4\pi c}{\hbar}]\) will suffice.

We quantize the variable \(p\) as above and, using the fact that \(p > 0\), we can define \(\hat{p} \equiv \left(-\frac{\hbar^2}{4\pi c^2} \partial_{x^2}\right)^{1/2}\), the volume operator \(\hat{V} \equiv \hat{p}^{1/2}\), and the scale factor \(\hat{a} \equiv \hat{p}^{1/2}\). The eigenfunctions of these operators are \(|n\rangle \equiv \sqrt{\frac{4\pi c}{\hbar}} e^{-\frac{4\pi n^2 c^2}{\hbar^2}}\), and their eigenvalues are \(|\hat{p}n\rangle = \frac{4\pi}{\hbar^3} \langle n|p|^2\rangle, (\hat{V}n) = \left(\frac{4\pi}{\hbar^3} |n|^2 \right)^{3/2}\) and \(|\hat{a}n\rangle = \sqrt{\frac{4\pi c}{\hbar}} e^{-\frac{4\pi n^2 c^2}{\hbar^2}}\). Using Eq. \(17\),

\[
\hat{a}^{-1} = -\frac{1}{4\pi c^2} Tr \sum_{j=1}^3 \sigma_j \hat{h}_j(1) [\hat{h}_j^{-1}(1), \hat{V}^{-1/3}],
\]

(25)
and consequently the corresponding quantum operator is
\[ \hat{a}^{-1} |n\rangle = \sqrt{\frac{3}{4\pi \ell_p^3}} \left( \sqrt{|n+1|} - \sqrt{|n-1|} \right) |n\rangle, \] (26)
whose eigenvalues, when \( n \gg 1 \), satisfy \( (\hat{a}^{-1})_n = 1/(\hat{a})_n \).

The quantization of the gravitational part of the Hamiltonian, depends on the order we fix. For instance, \( \hat{H}_{\text{grav},i} \equiv \frac{i\hbar}{2\pi \ell_p^3} \sum_{i,j,k} \varepsilon^{ijk} Tr \left[ \hat{h}_i^{-1}(1) \hat{h}_j^{-1}(1) \hat{h}_k^{-1}(1) \right] \) gives us a self-adjoint operator, or the direct quantization of the expression \( -\frac{\gamma^2 c^2 a \sin^2 \frac{\pi a}{2} \hat{a}}{2} \) yields
\[ \hat{H}_{\text{grav},i} = -\frac{\gamma^2 c^2}{2\ell_p^3} \hat{a}^{1/2} \sin^2 \left( \frac{\pi a}{2c} \right) \hat{a}^{1/2}. \] (27)
If we use this operator (27) as the gravitational part of the full Hamiltonian, then this is given by
\[ \hat{H}_i = -\frac{\gamma^2 c^2}{2\ell_p^3} \hat{a}^{1/2} \sin^2 \left( \frac{\pi a}{2c} \right) \hat{a}^{1/2} + \frac{1}{2\gamma^2} (\hat{a}^{-1})^3 \hat{p}_v^2, \] (28)
and in this case the WDW equation becomes \( \hat{H}_i \Phi = 0 \) which, expanding \( \Phi \) as \( \Phi = \sum_{n\in\mathbb{N}} \Phi_n(\psi) |n\rangle \), turns into
\[ 2\sqrt{|n|} \Phi_n - |n(n-4)|^{1/4} \Phi_{n-4} - |n(n+4)|^{1/4} \Phi_{n+4} \]
\[ +4 \left( \sqrt{|n+1|} - \sqrt{|n-1|} \right)^3 \partial_{\hat{p}_v}^3 \Phi_n = 0, \quad n \in \mathbb{N}. \] (29)

Summing up, the effective equation \( i\hbar \partial_t \Phi = \hat{H}_i \Phi \) with the condition \( \langle \hat{H}_i \phi(n) \rangle = 0 \) yields an average of the scalar factor operator that has essentially the same behavior as the classical solution of Eq. (20). This owes to the fact that the domain of the holonomy operators is the whole space, so that one can safely use the Heisenberg picture in order to obtain the quantum version of the classical equations. This gives generically small corrections to the classical behavior.

A final remark is in order. The singularity is avoided in the classical theory after regularization of the Hamiltonian. Quantization of this new Hamiltonian provides then a self-adjoint operator. It is important to realize that it is the regularization of the classical Hamiltonian what avoids the singularity, rather than the quantum effects. This is overlooked in some papers, where it is claimed that quantum effects are essential to avoid the big bang singularity \( [18, 23, 24] \). Note that in these approximations one already starts from the quantum theory and then, using the quantum operators an effective Hamiltonian is obtained \( [27, 28, 29] \) which, in fact, is in essence the Hamiltonian \( [18] \). This is maybe the reason why it is plainly concluded there that quantum effects, provided by LQC, are responsible for avoiding the big bang singularity. Here, with our alternative formulation we have shown, by means of explicit examples, that this need not be the case.

**IV. CONCLUSIONS**

We have presented here an effective formulation that naturally avoids the big bang singularity: in essence Schrödinger’s equation with the condition that the average of the Hamiltonian operator be zero. This is different from the Wheeler-DeWitt equation where one impose that the Hamiltonian operator annihilates the wave-function, and the arrow of time is yet to be selected. In our theory, physical time has essentially the same meaning as in the classical theory, and the relevant quantities are averages of quantum operators, as e.g. the average of the scale factor operator—which is by definition strictly positive—and no singularity appears at finite time. Our approach is remarkably natural (once time is assumed to exist), revolutionary and predictive, albeit rather non-trivial. It does not seem easy to produce an analytic formula that provides information on the behavior of the observable averages. Only numerical results look feasible at this point.

Another way to deal with the classical big bang singularity is LQC. We have here involved a simplified version of this theory and shown that, in contradistinction with the theory presented above, in LQC it is the regularization of the classical Hamiltonian that seems to avoid the singularity, and not the quantum effects obtained after quantization of the regularized Hamiltonian.

**V. APPENDIX A: SELF-ADJOINT EXTENSIONS OF SYMMETRIC OPERATORS**

In this mathematical Appendix we present a brief review of the theory of the self-adjoint extensions of symmetric operators.
Let \( \hat{A} \) be a linear operator that is defined on a dense subset \( D_\hat{A} \) of a separable Hilbert space \( \mathcal{H} \). The adjoint \( \hat{A}^\dagger \) of \( \hat{A} \) is defined on those vectors \( \Phi \in \mathcal{H} \) for which there exist \( \hat{\Phi} \in \mathcal{H} \) such that \( \langle \Phi | \hat{A} \Psi \rangle = \langle \hat{\Phi} | \Psi \rangle \) \( \forall \Psi \in D_\hat{A} \), and \( \hat{A}^\dagger \) is defined on such \( \Phi \) as \( \hat{A}^\dagger \Phi = \hat{\Phi} \).

The graph of an operator \( \hat{A} \) is a subset of \( \mathcal{H} \oplus \mathcal{H} \), defined by \( G_\hat{A} = \{(\Phi, \hat{\Phi}); \Phi \in D_\hat{A}\} \), and \( \hat{A} \) is called closed, which is written as \( \hat{A} = \hat{A} \), if its graph is a closed set. An extension of an operator \( \hat{A} \), namely \( \hat{A}_{\text{ext}} \), is an operator that satisfies \( D_\hat{A} \subset D_{\hat{A}_{\text{ext}}} \) and \( \hat{A}_{\text{ext}} \Phi = \hat{A} \Phi \) \( \forall \Phi \in D_\hat{A} \).

An operator \( \hat{A} \) is symmetric if \( \langle \Phi | \hat{A} \Psi \rangle = \langle \hat{A} \Phi | \Psi \rangle \) \( \forall \Phi, \Psi \in D_\hat{A} \). Then, a symmetric operator \( \hat{A} \) always admits a closure (a minimal closed extension), which is its double adjoint, i.e., \( \hat{A} = \hat{A}^{\dagger \dagger} \). The adjoint of a symmetric operator \( \hat{A} \) is always a closed extension of it, and it is self-adjoint when \( \hat{A} = \hat{A}^{\dagger \dagger} \). The deficiency subspaces \( \mathcal{N}_\pm \) of the operator \( \hat{A} \) are defined by

\[
\mathcal{N}_\pm = \left\{ \Phi \in D_{\hat{A}^{\dagger \dagger}}, \quad \hat{A}^\dagger \Phi = z_\pm \Phi, \quad \pm \text{Im}(z_\pm) > 0 \right\},
\]

and the deficiency indices \( n_\pm \) of \( \hat{A} \) are its dimensions. Note that, these two definitions do not depend on the values of \( z_\pm \).

The following theorem is due to Von Neumann:

For a closed symmetric operator \( \hat{A} \) with deficiency indices \( n_\pm \) there are three possibilities:

a) If \( n_+ = n_- = 0 \), then \( \hat{A} \) is self-adjoint.

b) If \( n_+ = n_- = n \geq 1 \), then \( \hat{A} \) has infinitely many self-adjoint extensions parametrized by an unitary \( n \times n \) matrix. Each unitary matrix \( U_n : \mathcal{N}_+ \rightarrow \mathcal{N}_- \), characterizes a self-adjoint extension \( \hat{A}_{U_n} \) as the restriction of \( \hat{A}^{\dagger \dagger} \) to the domain

\[
D_{\hat{A}_{U_n}} = \left\{ \Phi + \Phi_{z+} + U_n \Phi_{z+}; \Phi \in D_\hat{A} \quad \Phi_{z+} \in \mathcal{N}_+ \right\}.
\]

c) If \( n_+ \neq n_- \), then \( \hat{A} \) has no self-adjoint extensions.

### VI. APPENDIX B: EFFECTIVE FORMULATION FOR A BAROTROPIC PERFECT FLUID

In this Appendix we apply our effective formulation to the case of a barotropic perfect fluid with state equation \( p = \omega \rho \). The Lagrangian of the system in the flat case \( (k = 0) \) is

\[
L = -\frac{\gamma^2}{2} \dot{a}^2 a - \rho(a)a^3.
\]

The momentum and the Hamiltonian are respectively \( p_a = -\gamma^2 \dot{a} a \), and \( H = -\frac{1}{2\gamma^2} \dot{p}_a^2 + \rho(a)a^3 \). Using the conservation equation \( \dot{a} = -3H(\rho + p) \) we have \( \rho(a) = \rho_0 (a/a_0)^{-3(\omega+1)} \), then the dynamical equations become

\[
\dot{a} = -\frac{p_a}{\gamma^2 a}; \quad \ddot{p}_a = -\frac{p_a^2}{2\gamma^2 a^2} + 3\omega \rho(a)a^2,
\]

with the constraint \( H = 0 \).

The quantization rule \([3]\) give us the following Hamiltonian operator

\[
\hat{H} = \frac{\hbar^2}{2\gamma^2 a} \partial_a^2 + \rho(a)a^3,
\]

which is symmetric with respect to the inner product \( \langle \Phi | \Psi \rangle = \int_0^\infty da \Phi^\dagger(a)\Psi(a) \) of the Hilbert space \( L^2((0, \infty), ada) \).

To apply the theory presented in the Appendix A, first we consider the case \( \omega = 0 \) (dust matter), whose Hamiltonian is \( \hat{H} = \frac{\hbar^2}{2\gamma^2 a} \dot{a}^2 + \rho_0 a^3 \). To study the self-adjoint extensions of this operator we need to determine the deficiency subspaces \( \mathcal{N}_\pm \), that is, we must solve the equation \( \hat{H}\Phi = z_\pm \Phi \) with \( ||\Phi|| < \infty \). Since the definition of these spaces do not depend on \( z_\pm \), we choose, \( z_\pm = \pm i(\rho_0 a_0^3) \). Then the solutions of \( \hat{H}\Phi = \pm i(\rho_0 a_0^3) \Phi \) are the Airy’s functions \( \Phi_{\pm, a} \equiv A i(\beta_\pm a) \) and \( \Phi_{\pm, e} \equiv B i(\beta_\pm a) \), where \( \beta_\pm \equiv \left( \frac{\pi^2}{\pi^2 a^6} \right)^{1/3} e^{\pm i\pi/4} \). However, only \( \Phi_{1, e} \) has finite norm, and then both spaces has dimension 1. Von Neumann’s theorem says us that \( \hat{H} \) has infinitely many self-adjoint extensions, namely \( \hat{H}_{SA} \), parametrized by an unitary \( 1 \times 1 \) matrix, i.e., by \( e^{i\alpha} \) being \( \alpha \in \mathbb{R} \). To obtain an explicit expression of the domain of these self-adjoint extensions we must impose \([10, 31]\) \( \langle \hat{H}_{SA}(\Phi_+ + e^{i\alpha}\Phi_-) | \Psi \rangle = \langle \Phi_+ + e^{i\alpha}\Phi_- | \hat{H}_{SA} \Psi \rangle \forall \Psi \in D_{\hat{H}_{SA}} \). It is not difficult to show that, this condition is accomplished when

\[
\Psi(0) = \frac{A i(0) \Phi(0)}{\text{Im}(0) \beta_+} \equiv r, \quad \text{with} \quad r \in \mathbb{R}.
\]

\[
\Psi(0) = \frac{A i(0) \Phi(0)}{\text{Im}(0) \beta_+} \equiv r, \quad \text{with} \quad r \in \mathbb{R}.
\]
That is, for different values of $r$ we obtain different self-adjoint extensions. Here a very natural extension is obtained choosing $r = 0$, that is, imposing $\Psi(0) = 0$. Physically, this is equivalent to assume that at $a = 0$ there is a infinite potential barrier (in the same way that for no-relativistic one-dimensional barrier problems), then the existence of a solution all the time is guaranteed because when the scale factor decreases to zero, at some finite time, the potential barrier forces it to grow. Moreover, this assumption explains why the Heisenberg picture fails to work, because in the Heisenberg picture the boundary conditions do not appear, and the effective scale factor has the freedom to take all the values in $\mathbb{R}$, in particular, 0 or negative values. We can conclude that if we want to work in Heisenberg picture we must introduce some kind of potential barriers that prevent that the effective scalar factor takes negative values.

Once we have obtained a self-adjoint extension we apply the effective formulation (I) to the problem

$$i\hbar \partial_t \Phi(t) = \frac{\hbar^2}{2\gamma^2 a^2} \partial^2_x \Phi(t) + \rho_0 a^3 \Phi(t),$$

with the additional conditions $\Phi(t^*) = \Psi, \langle \hat{H}_{SA} \rangle = 0$, $||\Psi|| = 1$, that gives us a strongly continuous unitary one-parameter group defined on $L^2((0, \infty), ada)$ (Stone’s theorem), namely $e^{-\frac{i}{\hbar}H_{SA}t}$. The solution of our problem can be written as $\Phi(t) = e^{-\frac{i}{\hbar}H_{SA}(t-t^*)} \Psi$ for all $\Psi \in D\hat{H}_{SA}$ satisfying $\langle \hat{H}_{SA} \rangle = 0$ and $||\Psi|| = 1$. As an example of initial condition, if $r = 0$, one can take

$$\Psi(a) \equiv \frac{a^{-1}}{(\sigma \pi)^{1/4}} e^{-\frac{\ln^2(a/\bar{a})}{2\sigma}} e^{\frac{ia}{\hbar}(\ln(a/\bar{a})p^*)},$$

with $p^* = -\sqrt{2\rho_0 (a_0 \ddot{a})^3 \gamma e^{-2\sigma} - \hbar^2 (25/4 + 1/(2\sigma))}$. (36)

For this initial state, the effective scale factor $a_{eff}(t) = (\dot{a})_0 \Phi(\dot{a})$ grows forever for $t > t^*$ in the similar way to the classical one (the classical limit holds far of the turning point $a = 0$). For $t < t^*$ the effective scale factor decreases to zero, but at some finite time it bounces, due to the potential barrier, and then it grows to infinity.

Finally, we study the case $\omega = 1/3$ (radiation). The Hamiltonian is $\dot{H} = \frac{\hbar^2}{2\gamma^2 a^2} \partial^2_x + \frac{\rho_0 a^3}{\hbar}$, and the solutions of the equation $\dot{H} \Phi = \pm i \rho_0 a^3 \Phi$ are the Airy’s functions $\Phi_1, \Phi_2 \equiv A_i(\beta \pm (a \mp ia_0))$ and $\Phi_{2, \pm} \equiv B_i(\beta \pm (a \mp ia_0))$, where

$$\beta \equiv \left(\frac{2\gamma^2 \rho_0 a^3}{\hbar^2}\right)^{1/3} e^{i \pi/6}. $$

In this case the dimension of both deficiency subspaces is 1, then as the dust matter case, $\dot{H}$ has infinitely many self-adjoint extensions parametrized by an unitary $1 \times 1$ matrix, and the self-adjoint extensions are determined, once again, by the boundary condition $\Psi(0) = r \Psi'(0)$, with $r \in \mathbb{R}$. Now an initial condition for our effective formulation, that exhibits the same behavior as above for the effective scale factor, is given by the function

$$\Psi(a) \equiv \frac{a^{-1}}{(\sigma \pi)^{1/4}} e^{-\frac{\ln^2(a/\bar{a})}{2\sigma}} e^{\frac{ia}{\hbar}(\ln(a/\bar{a})p^*)},$$

with $p^* = -\sqrt{2\rho_0 (a_0 \ddot{a})^3 \gamma^2 e^{-2\sigma} - \hbar^2 (25/4 + 1/(2\sigma))}$. (37)

We finish this Appendix with the following remark. When the three-dimensional curvature is positive ($k = 1$), the Hamiltonian of the system is $\dot{H} = \frac{1}{2\gamma^2 a^2} \partial^2_x + \rho_0 a^3 (a^3 - \frac{1}{2}) \gamma^2 a$. Then the Hamiltonian constraint restricts the value of the scalar factor into the interval $(0, A)$ with $A = \left(\frac{2\rho_0 a_0^3 (3\omega + 1)}{(c\gamma)^2}\right)^{1/3}$, and this say us that we must take as Hilbert space, the space $L^2((0, A), ada)$. Now for $\omega \leq 1, a = 0$ is a regular singular point of the ordinary differential equation $\dot{H} \Phi = \pm \Phi$, then applying the Frobenius method we can deduce that there exist two independent solutions of the differential equation, consequently both deficiency indices are 2, because the domain $(0, A)$ is finite (excepts for $\omega = -1/3$). Then the self-adjoint extensions are parametrized by an unitary $2 \times 2$ matrix, and the more natural boundary condition is to assume that the wave-functions vanish at two boundary points. Physically this means that the scale factor is confined in a very deep well potential, and we have an oscillating universe whose effective scalar factor never vanishes.

VII. APPENDIX C: QFT IN CURVED SPACE-TIME FROM THE EFFECTIVE FORMULATION

For the flat FRW universe, the action that describes a massive scalar field conformally coupled with gravity in the presence of a barotropic fluid, is given by

$$S = \int_R dt \int_{[0, L]^3} d\vec{x} \left[ \frac{\gamma^2}{2} \dot{a}^2 a - \rho_0 (a/a_0)^{-3(\omega + 1)} a^3 + a^3 \mathcal{L}_\phi \right],$$

with $\mathcal{L}_\phi = \frac{1}{2hc} \dot{\phi}^2 - \frac{1}{2hc^2} (\nabla \phi)^2 - \frac{m^2}{2hc^2} \phi^2 - \frac{1}{12hc} R^2 \phi^2$ where $R = \frac{\delta}{\alpha_\gamma}(a_0^2 + a\ddot{a})$ is the scalar curvature. (Note that in this Appendix $\phi$ has energy units). Integrating with respect $\vec{x}$ and expanding $\phi$ in Fourier series ($\phi = \sum_{k \in \mathbb{Z}^3} \phi_k e^{2\pi i \vec{k} \cdot \vec{x}}$) one obtains,
\[ S = \int L(t) dt, \]

with

\[ L(t) = L^3 \left\{ -\frac{\alpha^2}{2} \nabla^2 a - \rho_0 (a/a_0)^{-3(\omega+1)} a^3 + a^3 \sum_{k \in \mathbb{Z}^3} \mathcal{L}_\phi \right\}, \tag{39} \]

where \( \mathcal{L}_\phi = \frac{1}{2 \hbar \sigma^2} \phi_k^2 - \frac{1}{2 \hbar \omega_a^2} \frac{4 \pi^2 |\vec{k}|^2 \phi_k^2}{L^2} - \frac{m^2 \sigma^2 \phi_k^2}{2 \hbar^2} - \frac{1}{12 \hbar c^2} R^2 \phi_k^2 \)

Using now the conformal time \( d\eta \equiv \frac{c t_p}{a} dt, \) (\( t_p \) being the Planck time) and defining the function \( \psi_\phi = \sqrt{\frac{4 \pi t_p}{3 \hbar}} \phi \), we obtain

\[ L(t) dt = \frac{4 \pi^2}{3 \hbar^2} \tilde{L}(\eta) d\eta, \]

with

\[ \tilde{L}(\eta) = -\frac{\hbar}{2t_p} \left( \frac{a'}{c} \right)^2 - \bar{\rho}_0 (a/a_0)^{-3(\omega+1)} \frac{a^4}{t_p} + \frac{1}{2} \sum_{k \in \mathbb{Z}^3} \left( \psi'_k \right)^2 - \frac{1}{t_p} \left[ \frac{4 \pi^2 |\vec{k}|^2}{L^2} + \left( \frac{a}{t_c} \right)^2 \right] \psi_k^2, \tag{40} \]

where we have introduced the Compton wavelengths \( l_c = \frac{h}{mc} \), and we have defined \( \bar{\rho}_0 = \frac{4 \pi}{3} \rho_0 \). The important remark should be made that in this Lagrangian we have suppressed the terms \( -\frac{\hbar^2}{m^2} \left( \frac{2}{a} \psi_k \right)' \).

The conjugate momenta are \( p_a = -\frac{\hbar}{t_p} a', p_{\psi_k} = \psi'_k \), and the Hamiltonian is given by

\[ \tilde{H}(\eta) = -\frac{1}{2m_p} p_a^2 + U(a) + \frac{1}{2} \sum_{k \in \mathbb{Z}^3} \left( p_{\psi_k}^2 + \omega_k^2(a) \psi_k^2 \right), \tag{41} \]

where \( m_p \) is the Planck mass and

\[ U(a) \equiv \bar{\rho}_0 (a/a_0)^{-3(\omega+1)} \frac{a^4}{t_p}, \quad \omega_k^2(a) \equiv \frac{1}{t_p^2} \left[ \frac{4 \pi^2 |\vec{k}|^2}{L^2} + \left( \frac{a}{t_c} \right)^2 \right]. \]

The quantum theory is obtained making the replacement \( p_a \rightarrow -i\hbar \partial_a \) and \( p_{\psi_k} \rightarrow -i\hbar \partial_{\psi_k} \). Then the quantum Hamiltonian is given by

\[ \hat{\tilde{H}} = \frac{\hbar^2}{2m_p} \partial_a^2 + U(a) + \hat{\tilde{H}}_m(a, \psi), \tag{42} \]

where the matter Hamiltonian is \( \hat{\tilde{H}}_m(a, \psi) = \sum_{k \in \mathbb{Z}^3} \left( \hbar \omega_k \hat{A}_k + \frac{1}{2} \hbar \omega_k^2 \right) \), where we have introduced the creation and annihilation operators

\[ \hat{A}_k^\dagger \equiv \frac{1}{\sqrt{2\hbar \omega_k}} (-\hbar \partial_{\psi_k} + \omega_k \psi_k); \quad \hat{A}_k \equiv \frac{1}{\sqrt{2\hbar \omega_k}} (\hbar \partial_{\psi_k} + \omega_k \psi_k). \tag{43} \]

Now, we show how one can obtain the QFT in curved space-time from the WDW equation. If we consider the matter field as a small perturbation, we look for solutions of the QFT equation with the form \( \Phi(a, \psi) = \Psi(a) \chi(a, \psi) \). After substitution in the WDW equation we obtain:

\[ \left[ \frac{\hbar^2}{2m_p} \partial_a^2 + U(a) \right] \chi + \left[ \Psi \frac{\hbar^2}{2m_p} \partial_a^2 \chi + \frac{\hbar^2}{m_p} \partial_a \Psi \partial_a \chi + \Psi \hat{\tilde{H}}_m \chi \right] = 0. \tag{44} \]

We assume at this point that \( \Psi \) is the solution of the equation

\[ -\frac{\hbar^2}{2m_p} \partial_a^2 \Psi - U(a) \Psi = 0, \tag{45} \]

and we make the change \( \Psi = e^{-\frac{a}{\hbar} S} \), then we obtain the system

\[ \begin{cases} \frac{(\partial_a S)^2}{2m_p} - U(a) + \frac{\hbar}{2m_p} \partial_a^2 S = 0 \\ \frac{\hbar^2}{2m_p} \partial_a^2 \chi - i \hbar \frac{\partial_a S}{m_p} \partial_a \chi + \hat{H}_m \chi = 0. \end{cases} \tag{46} \]
To solve this equations we neglect, as Rubakov does [32], the second derivative with respect to \(\alpha\), then we obtain the system

\[
\begin{cases}
\frac{\partial \phi}{2m_p} - U(\alpha) = 0 \\
-i\hbar \frac{\partial}{\partial m} \partial_a \chi + \dot{H}_m \chi = 0.
\end{cases}
\]

(47)

The first equation is the classical Hamilton-Jacobi equation, and the second one is the quantum Schrödinger equation that can be solved choosing as solution of the Hamilton-Jacobi equation \(S(\alpha) = \int_0^\alpha \sqrt{2m_pU(\alpha)} d\alpha\), and introducing the conformal time \(\frac{d\alpha}{d\tau} = \frac{\partial \phi}{2m_p}\), then the Schrödinger equation becomes \(i\hbar \partial_\tau \chi = \hat{H}_m(\alpha(\tau), \psi)\chi\).

Finally, we devise a method to obtain the QFT in curved space-time from the effective equation \(i\hbar \partial_\gamma \Phi = \tilde{H} \Phi\). Assuming that the matter field is a small perturbation, we look for solutions of the form \(\Phi(\alpha, \psi; \eta) = \hat{\Psi}(a; \eta) \chi(\psi; \eta)\) where \(\hat{\Psi}\) is the solution of the equation

\[
\hat{\Psi} - \frac{\hbar^2}{2m_p} \partial_a^2 \hat{\Psi} + U(\alpha) \hat{\Psi} = 0,
\]

and we assume that \(\hat{\Psi}\) is a function concentrated around a classical solution, namely \(a_c(\eta)\), of the following equation

\[
-\frac{1}{2m_p} \partial_a^2 + U(\alpha) = 0.
\]

(49)

By inserting \(\Phi\) in the effective equation one obtains \(\Psi i\hbar \partial_\gamma \chi = \Psi \dot{H}_m(\alpha, \psi)\chi\), and since \(\Psi\) is concentrated around the classical solution, one can approximate \(\Psi \dot{H}_m(\alpha, \psi)\chi\) by \(\Psi \hat{H}_m(a_c(\eta), \psi)\chi\), and then one obtains \(i\hbar \partial_\eta \chi = \hat{H}_m(a_c(\eta), \psi)\chi\).

We end with a last remark. From the effective formulation it’s not difficult to obtain the semi-classical Einstein equations. Effectively, starting with the condition \(\langle \dot{H}_m \rangle = 0\), if we take the wave function used above (now picked around \(a_c + \delta a_c\), one approximately obtain

\[
-\frac{1}{2m_p} \partial_a^2 + U(\alpha + \delta a_c) + \langle \dot{H}_m(a_c(\eta) + \delta a_c(\eta), \psi) \rangle_{\chi, \text{ren}} = 0,
\]

(50)

where the quantity \(\langle \dot{H}_m(a_c(\eta) + \delta a_c(\eta), \psi) \rangle_{\chi}\) has been renormalized.

Since \(a_c\) is solution of the equation [49], one also obtains, in the linear approximation, the following back-reaction equation:

\[
-\frac{\hbar}{c_{\text{pl}}} a_c' \delta a_c' + U'(a_c) \delta a_c + \langle \dot{H}_m(a_c(\eta), \psi) \rangle_{\chi, \text{ren}} = 0.
\]

(51)

Finally, observe that the derivation of the semi-classical Einstein equation from the WDW one is not a completely clear case (see for example [33]).

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[1] C. Molina-París and M. Visser, Phys. Lett. B455, 90 (1999); S.W. Hawking and R. Penrose, The nature of space and time, (Princeton Univ. Press, USA, 1996); S.W. Hawking and G.F.R. Ellis, The large scale structure of space-time (Cambridge, England, 1973).
[2] G.F.R. Ellis and R. Maartens, Class. Quantum Grav. 21, 223 (2004).
[3] G.F.R. Ellis, J. Murugan and C.G. Tsagas, Class. Quantum Grav. 21, 233 (2004).
[4] D.J. Mulryne, R. Tavakol, J.E. Lidsey and G.F.R. Ellis, Phys. Rev. D71, 123512 (2005).
[5] L. Parker and S.A. Fulling, Phys. Rev. D7, 2357 (1973).
[6] P.C.W. Davies, Phys. Lett. B68, 402 (1977).
[7] A.A. Starobinsky, Phys. Lett. B91, 99 (1980).
[8] B.S. DeWitt, Phys. Rev. 160, 1113 (1967).
[9] T. Thiemann, Introduction to modern canonical quantum general relativity, gr-qc/0110034 (2001).
[10] B.L. Voronov, D.M. Gitman and I.V. Tyutin, Rus. Phys. J. 50, 1 (2007).
[11] G. Bonneau, J. Faraut and V. Galiano, Am. J. Phys. 69, 322 (2001).
[12] A. Ashtekar, Nuovo Cim. B122, 135 (2007).
[13] M. Bojowald, Living Rev. Rel. 8, 1 (2005).
[14] C. Rovelli and L. Smolin, Phys. Rev. Lett. 72, 446 (1994).
[15] T. Thiemann, Class. Quantum Grav. 15, 1281 (1998).
[16] A. Ashtekar, M. Bojowald and J. Lewandowski, Adv. Theor. Math. 7, 233 (2003).
[17] A. Ashtekar, T. Pawlowski and P. Singh, Phys. Rev. Lett. 96, 141301 (2006).
[18] A. Ashtekar, T. Pawlowski and P. Singh, Phys. Rev. D73, 124038 (2006).
[19] V. Mukhanov, Physical Fundation of Cosmology, Cambridge University Press (2005).
[20] P. Singh and K. Vandersloot, Phys. Rev. D72, 084004 (2005).
[21] P. Singh, Phys. Rev. D73, 063508 (1976).
[22] M. Bojowald, Phys. Rev. Lett. 89, 261301 (2002).
[23] M. Bojowald, Phys. Rev. Lett. 86, 5227 (2001).
[24] M. Bojowald, Phys. Rev. Lett. 87, 121301 (2001).
[25] A. Ashtekar, T. Pawlowski, P. Singh and K. Vandersloot, Phys. Rev. D75, 024035 (2007).
[26] L. Szulc, W. Kaminski and J. Lewandowski, Class. Quantum Grav. 24, 2621 (2007).
[27] K. Vandersloot, Phys. Rev. D71, 103506 (2005).
[28] G. Date and G.M. Hossain, Class. Quantum Grav. 21, 4941 (2004).
[29] K. Banerjee and G. Date, Class. Quantum Grav. 22, 2017 (2005).
[30] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1972).
[31] V.S. Araujo, F.A.B. Coutinho and J.F. Perez, Am. J. Phys. 72, 203 (2003).
[32] V.A. Rubakov, JETP Lett. 39, 107 (1984); Phys. Lett. B29, 280 (1984).
[33] J.J. Halliwell, Phys. Rev. D36, 3626 (1987).