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An effective gravity model and singularity avoidance in quantum FRW cosmologies

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Abstract
An effective formulation of gravity is discussed, which lies in between the Wheeler–DeWitt approach and that of classical cosmology. It has the virtue of naturally avoiding the singularity that appears in Friedman–Robertson–Walker cosmologies. The mechanism is made explicit in specific examples, where it is compared with the quantization provided by loop quantum cosmology. It is argued that it is the regularization of the classical Hamiltonian, performed in that theory, that avoids the singularity, rather than usually invoked quantum effects. However, a deeper study of the quantum nature of geometry in that framework should help to completely clarify the issue.

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1. Introduction

Classical Friedman–Robertson–Walker (FRW) cosmologies give rise to a singularity when the strong-energy condition holds: $\rho + 3p > 0$, ρ being the energy density and p the pressure [1]. A simple way to avoid this singularity is by introducing a scalar field that breaks the strong-energy condition [2–4]. Another possibility is to consider quantum effects due to vacuum polarization, such as that due to a massless scalar field conformally coupled with gravity [5–7]. And still another approach is to consider quantum cosmological perfect fluid models in Schutz's formalism [8–10]. Here we will follow a different path, a modified gravity quantization stemming from the Wheeler–DeWitt equation: $\hat{H}\Phi = 0$

[11, 12], with $\hat{H}$ being the quantum Hamiltonian. To address the question of a possible singularity at finite time, we consider an effective formulation given in terms of the following Schrödinger equation (where we have chosen as time the cosmic one), with additional conditions:

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

We thus skip here, from the very beginning, the deep and fundamental question of the choice of a time direction [13], which we plainly assume to have a physical solution.

Some basic technical details on what will be demonstrated follow below. The quantum Hamiltonian $\hat{H}$, obtained with the usual rules of quantum mechanics, is generically symmetric but not self-adjoint. Von Neumann's theorem [14, 15] allows it to be extended (sometimes in infinitely many ways) to a self-adjoint operator. 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: $a_{\text{eff}}(t) \equiv \langle\Phi(t)|\hat{a}\Phi(t)\rangle$, 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 infinite barrier potential at the point $a = 0$, then when the effective factor scales approach to zero, at some finite time, it bounces and grows.

However, to compute averages one usually works in the Heisenberg picture, so $\dot{\hat{A}} = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{A}]$, for $\hat{A}$ 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 scalar 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, which invalidates the final result (physically, one can explain this taking into account that in the Heisenberg picture the boundary conditions do not appear, i.e., the barrier potential is 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 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 [16, 17]. In what follows, we present a simple demonstration of the above approach and will explicitly see how this theory avoids the singularity. It will also be shown that it is the regularization of the classical Hamiltonian [18–20] that avoids the singularity, rather than quantum effects.

In the first of the three appendices in the article 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 one 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 extension of the respective Hamiltonian operators can be understood assuming that there is an infinite potential barrier at $a = 0$. Finally, in the last one, we show (resp. review) how to derive the standard quantum fields theory in curved spacetime from the effective formulation (resp. the Wheeler–DeWitt equation), and also we obtain, from the effective formulation, the semi-classical Einstein equation, that is, the back-reaction one.

2. The problem

In this section, we consider a homogeneous and isotropic gravitational field minimally coupled to a homogeneous scalar field, the Lagrangian of which is given by [4]

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

where G is Newton's constant, and k is the three-dimensional curvature. We are interested in the case $k = 0$ and $V \equiv 0$, previously studied in [21, 22] within the framework of LQC. This interest comes from the fact that in the chaotic inflationary model with $V = \frac{1}{2}m^2\phi^2$, at very early times before the inflationary period, one has $\dot{\phi} \gg V$ (for details, see [23]). Then the potential can be neglected and one has $\rho \cong p$. Consequently, this model gives 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 ψ by $\phi = \sqrt{3c^2/4\pi G}\psi$, the Lagrangian becomes (l_p denotes the Planck length)

$$L = -\frac{\gamma^2}{2}(\dot{a}^2a - \dot{\psi}^2a^3), \qquad \text{with} \qquad \gamma^2 = \frac{3c^2}{4\pi G} = \frac{3\hbar}{4\pi c l_p^2}. \tag{3}$$

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

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

The classical dynamic equations are

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

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

$$\begin{aligned} &0 > a(t)p_a(t) \equiv p_\alpha^*, \qquad p_{\psi;\pm}(t) \equiv p_{\psi,\pm}^* = \pm p_\alpha^*, \\ &a(t) = a^*\left[1 - \frac{3p_\alpha^*(t-t^*)}{\gamma^2(a^*)^3}\right]^{1/3}, \qquad \psi_\pm(t) = \mp\ln\frac{a(t)}{a^*} + \psi^*. \end{aligned} \tag{6}$$

Note that the solution $(a(t), \psi_\pm(t))$ is defined in the interval $(t_s, +\infty)$, where $t_s = t^* + (\gamma^2/3p_\alpha^*)(a^*)^3$. 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 $a(t) = a^*[1 - (t - t^*)/(t_s - t^*)]^{1/3}$. Finally, from equations (5) we have $\mathrm{d}\ln a/\mathrm{d}\psi_\pm = \mp 1$ and conclude that

$$a = a^*\,\mathrm{e}^{\mp(\psi_\pm - \psi^*)}. \tag{7}$$

2.1. Quantum dynamics

We now use the quantization rule,

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

and obtain the quantum Hamiltonian,

$$\hat{H} \equiv \frac{\hbar^2}{2\gamma^2a^3}\left(a\partial_a a\partial_a - \partial_{\psi^2}^2\right). \tag{9}$$

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

$$\begin{aligned} \frac{\mathrm{d}\hat{a}}{\mathrm{d}t} &= -\frac{1}{\gamma^2\hat{a}^2}(\widehat{ap}_a + \mathrm{i}\hbar), & \frac{\mathrm{d}(\widehat{ap}_a)}{\mathrm{d}t} &= 3\hat{H}, \\ \frac{\mathrm{d}\hat{\psi}}{\mathrm{d}t} &= \frac{1}{\gamma^2\hat{a}^3}\hat{p}_\psi, & \frac{\mathrm{d}\hat{p}_\psi}{\mathrm{d}t} &= 0, \end{aligned} \tag{10}$$

with $\langle\Phi|\Psi\rangle \equiv \int_0^\infty \mathrm{d}a \int_{\mathbb{R}} \mathrm{d}\psi\, \Phi^*(a,\psi)a^2\Psi(a,\psi)$ as the inner product and operator average $\langle\hat{A}\rangle_\Psi \equiv \langle\Psi|\hat{A}\Psi\rangle$, $\|\Psi\| = 1$.

Example 1. Consider the wavefunction ($|p_\alpha^*| = |p_\psi^*|$): $\Psi(a,\psi) \equiv \frac{a^{-3/2}}{(\sigma\pi)^{1/2}}\mathrm{e}^{-\frac{\ln^2(a/\bar{a})}{2\sigma}}\mathrm{e}^{-\frac{(\psi-\psi^*)^2}{2\sigma}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\ln(a/\bar{a})p_\alpha^* + \psi p_\psi^*)}$. Then: $\langle\hat{a}\rangle_\Psi = \bar{a}\,\mathrm{e}^{\sigma/4} \equiv a^*$, $\langle\hat{\psi}\rangle_\Psi = \psi^*$, $\langle\widehat{ap_a}\rangle_\Psi = p_\alpha^*$, $\langle\hat{p}_\psi\rangle_\Psi = p_\psi^*$ and $\langle\hat{H}\rangle_\Psi = 0$.

2.2. *The Wheeler–DeWitt equation*

Compare at this point with the Wheeler–DeWitt equation paradigm (WDW) [11],

$$\hat{H}\Phi = 0 \longrightarrow \big(a\partial_a a\partial_a - \partial^2_{\psi^2}\big)\Phi = 0, \tag{11}$$

with the general solution ($\widetilde{a}$ is a length constant)

$$\Phi(a,\psi) = f_+(\ln(a/\widetilde{a}) + \psi) + f_-(\ln(a/\widetilde{a}) - \psi). \tag{12}$$

The quantum version of equation (7) is $\Phi_+(a,\psi) = f_+(\ln(a/a^*) + \psi - \psi^*)$, $\Phi_-(a,\psi) = f_-(\ln(a/a^*) - \psi + \psi^*)$, with $f_\pm$ being a function picked around 0, as, for instance, $f_\pm(z) = \mathrm{e}^{-z^2/\sigma}$. 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 (1). Note that $\langle\hat{H}\rangle_\Psi = 0$ implies $\langle\hat{H}\rangle_{\Phi(t)} = 0$, and $\|\Psi\| = 1$ implies $\|\Phi(t)\| = 1, \forall t \in \mathbb{R}$. Then, if the solution of the problem exists for all t, it is easy to prove that the effective scalar factor, $a_{\mathrm{eff}}(t) \equiv \langle\hat{a}\rangle_{\Phi(t)}$, never vanishes. In fact, the condition $\|\Psi\| = 1$ implies $\|\Phi(t)\| = 1$, i.e., $\int_0^\infty \mathrm{d}a \int_{\mathbb{R}} \mathrm{d}\psi\, a^2|\Phi(t,a,\psi)|^2 = 1$, and thus we have $a_{\mathrm{eff}}(t) = \langle\hat{a}\rangle_{\Phi(t)} = \int_0^\infty \mathrm{d}a \int_{\mathbb{R}} \mathrm{d}\psi\, a^3|\Phi(t,a,\psi)|^2 \neq 0$.

To do the calculation, we consider the quantity $\langle\hat{a}^3\rangle_{\Phi(t)}$. We have $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{a}^3\rangle_{\Phi(t)} = \frac{\mathrm{i}}{\hbar}\langle[\hat{H},\hat{a}^3]\rangle_{\Phi(t)} = -\frac{3}{\gamma^2}\langle\widehat{ap_a}\rangle_{\Phi(t)}$ and $\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\hat{a}^3\rangle_{\Phi(t)} = -\frac{3\mathrm{i}}{\hbar\gamma^2}\langle[\hat{H},\widehat{ap_a}]\rangle_{\Phi(t)} = -\frac{9}{\gamma^2}\langle\hat{H}\rangle_{\Phi(t)} = 0$, due to the remark above. Consequently, we obtain

$$\langle\hat{a}^3\rangle_{\Phi(t)} = \langle\hat{a}^3\rangle_\Psi - \frac{3}{\gamma^2}\langle\widehat{ap_a}\rangle_\Psi(t - t^*). \tag{13}$$

For the function of example 1, we get

$$\langle\hat{a}^3\rangle_{\Phi(t)} = \bar{a}^3\mathrm{e}^{9\sigma/4} - \frac{3}{\gamma^2}p_\alpha^*(t - t^*), \tag{14}$$

and this contradicts the fact that $\langle\hat{a}^3\rangle_{\Phi(t)} \geqslant 0, \forall t \in \mathbb{R}$. However, since the operator $\hat{H}$ is symmetric and real, using von Neumann's theorem [14, 15] it can be extended to a self-adjoint one, and then the solution of the problem (1) 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 $[\hat{H},\widehat{ap_a}]$ 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. Before using it in our problem, we consider another example where the above contradictions can easily be depicted.

Example 2. Consider now the problem,

$$\mathrm{i}\partial_t\Phi = -\mathrm{i}\hbar c\partial_x\Phi \equiv c\hat{p}\Phi, \qquad \forall x\in[0,2\pi], \qquad \Phi(0)=\Psi, \tag{15}$$

$\hat{p}$ being the self-adjoint in the domain [15]: $D_{\hat{p}} = \{\Psi$ absolutely continuous in $[0,2\pi]$, $\partial_x\Psi \in \mathcal{L}^2[0,2\pi]$, $\Psi(0)=\Psi(2\pi)\}$. Let $\Phi(t)$ be the solution of our effective formulation (15). We want to calculate $\langle\hat{x}\rangle_{\Phi(t)} \equiv \int_0^{2\pi} x|\Phi(t,x)|^2\,\mathrm{d}x$. Using $[\hat{p},\hat{x}] = -\mathrm{i}\hbar$, we get $\langle\dot{\hat{x}}\rangle_{\Phi(t)} = c$, i.e., $\langle\hat{x}\rangle_{\Phi(t)} = \langle\hat{x}\rangle_\Psi + ct$ which is *not* positive $\forall\, t$. What actually happens is that, for some t, we have $\hat{x}\Phi(t)\notin D_{\hat{p}}$, and then $\hat{p}\hat{x}\Phi(t)$ has no sense, neither the formula $\langle\dot{\hat{x}}\rangle_{\Phi(t)} = \frac{\mathrm{i}}{\hbar}\langle[c\hat{p},\hat{x}]\rangle_{\Phi(t)}$. To see this in detail, consider the initial state

$$\Psi(x) = \sqrt{\frac{3}{2\pi^2}}\begin{cases} x, & \text{for} \quad x\in[0,\pi],\\ 2\pi - x, & \text{for} \quad x\in[\pi,2\pi].\end{cases} \tag{16}$$

Fourier analysis provides the following solution of the Schrödinger equation:

$$\Phi(t,x) = \sqrt{\frac{3}{2\pi^2}}\left\{\frac{\pi}{2} - \frac{4}{\pi}\sum_{n\in\mathbb{Z}}\frac{1}{(2n+1)^2}\cos[(2n+1)(x-ct)]\right\}. \tag{17}$$

Then, at $t=0$ we have $x\Phi(0,x)\in D_{\hat{p}}$ but if we choose $t=\pi/c$, we obtain $x\Phi(\pi/c,x)|_{x=0} = 0$, and $x\Phi(\pi/c,x)|_{x=2\pi} = \sqrt{6}\pi/c$, which means effectively that $x\Phi(\pi/c,x)\notin D_{\hat{p}}$. However, note that $\langle\hat{x}\rangle_{\Phi(t)}$ exists for all $t\in\mathbb{R}$, its value being

$$0 < \langle\hat{x}\rangle_{\Phi(t)} = \int_0^{2\pi}\frac{3x}{2\pi^2}\left\{\frac{\pi}{2} - \frac{4}{\pi}\sum_{n\in\mathbb{Z}}\frac{1}{(2n+1)^2}\cos\left[(2n+1)(x-ct)\right]\right\}^2\mathrm{d}x < 2\pi. \tag{18}$$

3. Loop quantum cosmology to the rescue

We shall now involve (a simplified version of) LQC (for a rigorous formulation, see [17, 20]), 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 $x\equiv\dot{a}$. Their Poisson bracket is $\{x,p\} = \frac{8\pi G}{3c^2} = \frac{2}{\gamma^2}$. We also consider the holonomies $h_j(n)\equiv \mathrm{e}^{-\mathrm{i}\frac{n\iota x}{2c}\sigma_j} = \cos\left(\frac{n\iota x}{2c}\right) - \mathrm{i}\sigma_j\sin\left(\frac{n\iota x}{2c}\right)$ [25], where σ_j are the Pauli matrices, and ι is the Barbero–Immirzi parameter. We easily obtain the following classical identity of the Ashtekar–Barbero phase space [25]:

$$a^{-1} = \frac{-\mathrm{i}\hbar}{4\pi l_p^2\iota}\,\mathrm{Tr}\sum_{j=1}^{3}\sigma_j h_j(1)\left\{h_j^{-1}(1),a\right\}. \tag{19}$$

To get the gravitational part of the Hamiltonian, we cannot directly use this one: $H_{\text{grav}} = -\frac{3c^2}{8\pi G}x^2\sqrt{p}$, which leads to singular classical dynamics. We may use the general formulae of loop quantum gravity (LQG) to obtain the regularized Hamiltonian [12, 20, 22]:

$$\begin{aligned} H_{\text{grav},\iota} &\equiv -\frac{\hbar^2 c}{32\pi^2 l_p^4\iota^3}\sum_{i,j,k}\varepsilon^{ijk}\,\mathrm{Tr}\left[h_i(1)h_j(1)h_i^{-1}(1)h_j^{-1}(1)h_k(1)\left\{h_k^{-1}(1),a^3\right\}\right]\\ &= -\frac{\gamma^2c^2}{2\iota^2}a\sin^2\frac{\iota x}{c}, \end{aligned} \tag{20}$$

which is bounded when the extrinsic curvature $x/2$ (a half of the velocity of the scalar factor) diverges and approaches H_{grav} for small values of x. Then, taking this regularized Hamiltonian as the gravitational part of the full one, the last is given by [24, 25]

$$H_\iota \equiv -\frac{\gamma^2 c^2}{2\iota^2} a \sin^2 \frac{\iota x}{c} + \frac{1}{2\gamma^2} a^{-3} p_\psi^2, \tag{21}$$

and the dynamical equations are

$$\dot{a} = \{a, H_\iota\} = \frac{c}{2\iota} \sin \frac{2\iota x}{c}, \qquad \dot{x} = \{x, H_\iota\} = -\frac{2}{\gamma^2 a^4} p_\psi^2. \tag{22}$$

Imposing the Hamiltonian constraint $H_\iota = 0$, we obtain

$$\dot{a}^2 = \frac{p_\psi^2}{\gamma^4 a^4} \left(1 - \frac{p_\psi^2 \iota^2}{\gamma^4 a^4 c^2}\right), \tag{23}$$

and since $p_\psi \equiv p_\psi^*$ is constant, we get the following bounce: $\dot{a} = 0$ when $a = \frac{1}{\gamma}\sqrt{\frac{p_\psi^* \iota}{c}} = 2l_p\sqrt{\frac{\pi p_\psi^* \iota}{3\hbar}}$. Consequently, there is no singularity because the range of $a(t)$ is $\left[2l_p\sqrt{\frac{\pi p_\psi^* \iota}{3\hbar}}, +\infty\right), \forall t \in \mathbb{R}$. 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 [26], namely, from the Friedmann equation (23): $\ddot{a} > 0$, for $a \in \left(2l_p\sqrt{\frac{\pi p_\psi^* \iota}{3\hbar}}, 2l_p\sqrt{\frac{\sqrt{2}\pi p_\psi^* \iota}{3\hbar}}\right)$. Finally, note that when $a \gg l_p$, equation (23) coincides with (5).

A different way to understand these features is to write equation (23) as $\left(\frac{\dot{a}}{a}\right)^2 = \frac{2}{\gamma^2}\rho_{\text{eff}}$, where we have introduced the effective energy density $\rho_{\text{eff}} \equiv \frac{p_\psi^2}{2a^6}\left(1 - \frac{p_\psi^2 \iota^2}{\gamma^4 a^4 c^2}\right)$. 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 $p_{\text{eff}} \equiv \frac{p_\psi^2}{2a^6}\left(1 - \frac{7p_\psi^2 \iota^2}{3\gamma^4 a^4 c^2}\right)$. But then 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 $\left(2l_p\sqrt{\frac{\pi p_\psi^* \iota}{3\hbar}}, 2l_p\sqrt{\frac{\sqrt{2}\pi p_\psi^* \iota}{3\hbar}}\right)$, consequently, the singularity is avoided. Moreover, for $a \in \left(2l_p\sqrt{\frac{\pi p_\psi^* \iota}{3\hbar}}, 2l_p\sqrt{\frac{\sqrt{5}\pi p_\psi^* \iota}{3\sqrt{3}\hbar}}\right)$, there is a period of super-inflation, that is, in this interval, one has $\frac{p_{\text{eff}}}{\rho_{\text{eff}}} < -1$.

We should remark here that similar results are obtained in the case $k = 1$ and $V \equiv 0$. Now the classical Hamiltonian is given by

$$H = \frac{1}{2\gamma^2 a^3}\left(-(ap_a)^2 + p_\psi^2 - \gamma^4 c^2 a^4\right), \tag{24}$$

and the regularized one is

$$H_\iota \equiv -\frac{\gamma^2 c^2}{2\iota^2} a \left(\sin^2\left(\frac{\iota x}{c}\right) + \iota^2\right) + \frac{1}{2\gamma^2} a^{-3} p_\psi^2. \tag{25}$$

Then, using the Hamiltonian constraint, $H_\iota = 0$, it is easy to obtain the Friedmann equation

$$\dot{a}^2 = \left(\frac{p_\psi^2}{\gamma^4 a^4} - c^2\right)\left(1 + \iota^2 - \frac{p_\psi^2 \iota^2}{\gamma^4 a^4 c^2}\right), \tag{26}$$

and since $p_\psi \equiv p_\psi^*$ is constant and $\dot{a}^2 \geqslant 0$, we can deduce that $a \in \left[2l_p\sqrt{\frac{\pi p_\psi^* \iota}{3\hbar\sqrt{1+\iota^2}}}, 2l_p\sqrt{\frac{\pi p_\psi^*}{3\hbar}}\right]$, 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 $\widetilde{x} \equiv \dot{a} + c$; then following [29, 30], we obtain the regularized Hamiltonian,

$$\widetilde{H}_\iota \equiv -\frac{\gamma^2 c^2}{2\iota^2} a \left(\sin^2 \left(\frac{\iota(\widetilde{x} - c)}{c} \right) - \sin^2(\iota) + 2\iota^2 \right) + \frac{1}{2\gamma^2} a^{-3} p_\psi^2. \tag{27}$$

It is clear that from this last regularized Hamiltonian the scale factor has the same behavior as that described in equation (26).

3.1. Quantization

To quantize we perform the usual change $\{A, B\} \rightarrow -\frac{\mathrm{i}}{\hbar}[\hat{A}, \hat{B}]$. Note that the system is $\frac{4\pi c}{\iota}$-periodic with respect to the variable x; thus we consider the space of $\frac{4\pi c}{\iota}$-periodic functions and introduce the inner product $\langle \Psi | \Phi \rangle \equiv \int_{\mathbb{R}} \mathrm{d}\psi \int_{-\frac{2\pi c}{\iota}}^{\frac{2\pi c}{\iota}} \mathrm{d}x\, \Psi^*(x, \psi)\Phi(x, \psi)$. The completion of this space with respect to this product is the space of square-integrable functions in $\left[-\frac{2\pi c}{\iota}, \frac{2\pi c}{\iota}\right]$. Note that, rigorously, the definition of the Hilbert space is more complicated: $\mathcal{L}^2(\mathbb{R}_{\mathrm{Bohr}}, d\mu_{\mathrm{Bohr}})$, where $\mathbb{R}_{\mathrm{Bohr}}$ is the compactification of $\mathbb{R}$, and μ_{Bohr} is the Haar measure on it [22]. However, for our purposes the Hilbert space $\mathcal{L}^2\left[-\frac{2\pi c}{\iota}, \frac{2\pi c}{\iota}\right]$ will suffice.

We quantize the variable p as above and, using the fact that $p > 0$, we can define $\hat{p} \equiv \left(-\frac{4\hbar^2}{\gamma^4}\partial_{x^2}^2\right)^{1/2}$, the volume operator $\hat{V} \equiv \hat{p}^{3/2}$ and the scale factor $\hat{a} \equiv \hat{p}^{1/2}$. The eigenfunctions of these operators are $|n\rangle \equiv \sqrt{\frac{\iota}{4\pi c}}\, \mathrm{e}^{\frac{\mathrm{i}n\iota}{2c}x}$, and their eigenvalues that due to the choice of our Hilbert space are discrete are $(\hat{p})_n = \frac{4\pi}{3}\iota|n|l_p^2$, $(\hat{V})_n = \left(\frac{4\pi}{3}\iota|n|l_p^2\right)^{3/2}$ and $(\hat{a})_n = \sqrt{\frac{4\pi}{3}\iota|n|}l_p$. Since the spectrum of the scale factor is discrete, we can obtain different non-singular spectra of its inverse; for example, using equation (19),

$$\hat{a}^{-1} \equiv -\frac{1}{4\pi l_p^2 \iota} \operatorname{Tr} \sum_{j=1}^{3} \sigma_j \hat{h}_j(1)\left[\hat{h}_j^{-1}(1), \hat{V}^{1/3}\right], \tag{28}$$

one gets

$$\hat{a}^{-1}|n\rangle = \sqrt{\frac{3}{4\pi\iota}} \frac{1}{l_p}(\sqrt{|n+1|} - \sqrt{|n-1|})|n\rangle, \tag{29}$$

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, $\hat{H}_{\mathrm{grav},\iota} \equiv \frac{\mathrm{i}\hbar c}{32\pi^2 l_p^4 \iota^3} \sum_{i,j,k} \varepsilon^{ijk} \operatorname{Tr}\left[\hat{h}_i^{-1}(1)\hat{h}_j^{-1}(1)\hat{h}_k(1)\left[\hat{h}_k^{-1}(1), \hat{V}\right]\hat{h}_i(1)\hat{h}_j(1)\right]$ gives us a self-adjoint operator, or the direct quantization of the expression $-\frac{\gamma^2 c^2}{2\iota^2} a \sin^2 \frac{\iota x}{c}$ yields

$$\widehat{\widehat{H}}_{\mathrm{grav},\iota} \equiv -\frac{\gamma^2 c^2}{2\iota^2} \hat{a}^{1/2} \sin^2\left(\frac{\iota x}{c}\right)\hat{a}^{1/2}. \tag{30}$$

If we use this operator (30) as the gravitational part of the full Hamiltonian, then this is given by

$$\widehat{\widehat{H}}_\iota \equiv -\frac{\gamma^2 c^2}{2\iota^2} \hat{a}^{1/2} \sin^2\left(\frac{\iota x}{c}\right)\hat{a}^{1/2} + \frac{1}{2\gamma^2}(\hat{a}^{-1})^3 \hat{p}_\psi^2, \tag{31}$$

and in this case the WDW equation becomes $\widehat{\widehat{H}}_\iota \Phi = 0$ which, expanding Φ as $\Phi = \sum_{n\in\mathbb{N}} \Phi_n(\psi)|n\rangle$, turns into

$$2\sqrt{|n|}\Phi_n - |n(n-4)|^{1/4}\Phi_{n-4} - |n(n+4)|^{1/4}\Phi_{n+4} \\ +4(\sqrt{|n+1|} - \sqrt{|n-1|})^3 \partial^2_{\psi^2}\Phi_n = 0, \qquad n \in \mathbb{N}. \tag{32}$$

Summing up, the effective equation $\mathrm{i}\hbar\partial_t\Phi = \widehat{\widehat{H}}_\iota\Phi$ with the condition $\langle\widehat{\widehat{H}}_\iota\rangle_{\Phi(t)} = 0$ yields an average of the scalar factor operator that has essentially the same behavior as the classical solution of equation (23). This is due 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 the 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 [22, 27, 28]. Note that, in these approximations, one already starts from the quantum theory, and then using the quantum operators an effective Hamiltonian is obtained [31–33] which, in fact, is in essence the Hamiltonian (21). This may be the reason why it is plainly concluded there that quantum effects, provided by LQC, are responsible for avoiding the big bang singularity. However, it is very possible that a deeper study of the quantum nature of the geometry could actually resolve the singularities. But from our viewpoint, the discrete spectrum of the factor scale operator comes naturally from the fact that the regularized Hamiltonian is periodic. Here, with our alternative formulation we have shown, by means of explicit examples, that this need not be the case in other situations.

4. Conclusions

We have presented an effective formulation that avoids the big bang singularity: in essence Schrödinger's equation with the condition that the average of the Hamiltonian operator is zero. This is different from the Wheeler–DeWitt equation where one imposes that the Hamiltonian operator annihilates the wavefunction, and the time arrow is yet to be selected. In our theory, time has the same meaning as in the classical theory, and the relevant quantities are averages of the quantum operators, as, e.g., the average of the scale factor operator—which is by definition strictly positive—and there appears *no singularity at finite time*. The problem with this effective theory is that one cannot use Heisenberg's picture to calculate those quantities, and since it is also impossible to explicitly solve Schrödinger's equation, it does not seem easy to produce an analytic formula that gives us information on the behavior of these averages. Only numerical results look feasible at this point.

Another way to deal with the classical big bang singularity is LQC. We have considered here a simplified version of this theory and shown that, in contradistinction to 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 the quantization of the regularized Hamiltonian.

We should finally stress that our contribution is in no way a universal procedure trying to compete with fundamental quantizations of gravity, such as LQG or the WdW equation. It is just an effective, intermediate approach, simple and with some good properties. It deals with particular issues only, but can be fruitfully used at an intermediate cosmological level. The specific examples we have presented already hint toward this possibility.

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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 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 $\widetilde{\Phi} \in \mathcal{H}$ such that $\langle\Phi|\hat{A}\Psi\rangle = \langle\widetilde{\Phi}|\Psi\rangle \forall\, \Psi \in D_{\hat{A}}$, and $\hat{A}^\dagger$ is defined on such Φ as $\hat{A}^\dagger\Phi \equiv \widetilde{\Phi}$. The graph of an operator $\hat{A}$ is a subset of $\mathcal{H}\bigoplus\mathcal{H}$, defined by $G_{\hat{A}} \equiv \{(\Phi, \hat{A}\Phi);\ \Phi \in D_{\hat{A}}\}$, and $\hat{A}$ is called closed, which is written as $\bar{\hat{A}} = \hat{A}$, if its graph is a closed set. An extension of an operator $\hat{A}$, namely $\hat{A}_{\mathrm{ext}}$, is an operator that satisfies $D_{\hat{A}} \subset D_{\hat{A}_{\mathrm{ext}}}$ and $\hat{A}_{\mathrm{ext}}\Phi = \hat{A}\Phi \forall\, \Phi \in D_{\hat{A}}$.

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

$$\mathcal{N}_\pm = \{\Phi \in D_{\hat{A}^\dagger},\ \hat{A}^\dagger\Phi = z_\pm\Phi, \pm\mathrm{Im}(z_\pm) > 0\}, \tag{A.1}$$

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 important theorem holds.

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

$$D_{\hat{A}_{U_n}} = \left\{\Phi + \Phi_{z_+} + U_n\Phi_{z_+};\ \Phi \in D_{\hat{A}},\ \Phi_{z_+} \in \mathcal{N}_+\right\}. \tag{A.2}$$

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

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 the equation of state $p = \omega\rho$. The Lagrangian of the system in the flat case ($k = 0$) is

$$L = -\frac{\gamma^2}{2}\dot{a}^2 a - \rho(a)a^3. \tag{B.1}$$

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

$$\dot{a} = -\frac{p_a}{\gamma^2 a}; \qquad \dot{p}_a = -\frac{p_a^2}{2\gamma^2 a^2} + 3\omega\rho(a)a^2, \tag{B.2}$$

with the constraint $H = 0$. The quantization rule (8) gives us the following Hamiltonian operator:

$$\hat{H} = \frac{\hbar^2}{2\gamma^2 a}\partial_a^2 + \rho(a)a^3, \tag{B.3}$$

which is symmetric with respect to the inner product $\langle\Phi|\Psi\rangle = \int_0^\infty \mathrm{d}a\, a\Phi^*(a)\Psi(a)$ of the Hilbert space $\mathcal{L}^2((0,\infty), a\mathrm{d}a)$.

To apply the theory presented in appendix A, first we consider the case $\omega = 0$ (dust matter), whose Hamiltonian is $\hat{H} = \frac{\hbar^2}{2\gamma^2 a}\partial_a^2 + \rho_0 a_0^3$. 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 definitions of these spaces do not depend on $z_\pm$, we choose, $z_\pm = \pm\mathrm{i}\rho_0 a_0^3$. Then, the solutions of $\hat{H}\Phi = \pm\mathrm{i}\rho_0 a_0^3\Phi$ are Airy functions $\Phi_{1,\pm} \equiv Ai(\beta_\pm a)$ and $\Phi_{2,\pm} \equiv Bi(\beta_\pm a)$, where $\beta_\pm \equiv \left(\frac{4\gamma^2\rho_0 a_0^3}{\hbar^2}\right)^{1/3} \mathrm{e}^{\pm\mathrm{i}\pi/4}$ [34]. However, only $\Phi_{1,\pm}$ has finite norm, and then both spaces have dimension 1. Von Neumann's theorem tells us that $\hat{H}$ has infinitely many self-adjoint extensions, namely $\hat{H}_{\mathrm{SA}}$, parametrized by a unitary 1×1 matrix, i.e., by e^{α} being $\alpha \in \mathbb{R}$. To obtain an explicit expression of the domain of these self-adjoint extensions we must impose [14, 35] $\langle\hat{H}_{\mathrm{SA}}(\Phi_+ + \mathrm{e}^{\mathrm{i}\alpha}\Phi_-)|\Psi\rangle = \langle\Phi_+ + \mathrm{e}^{\mathrm{i}\alpha}\Phi_-|\hat{H}_{\mathrm{SA}}\Psi\rangle \forall\,\Psi \in D_{\hat{H}_{\mathrm{SA}}}$. It is not difficult to show that this condition is fulfilled when

$$\frac{\Psi(0)}{\Psi'(0)} = \frac{Ai(0)}{Ai'(0)|\beta_+|}\frac{1}{1+\tan(\alpha/2)} \equiv r, \qquad \text{with} \quad r \in \mathbb{R}. \tag{B.4}$$

That is, for different values of r we obtain different self-adjoint extensions. Here a very natural extension is obtained by choosing $r = 0$, that is, imposing $\Psi(0) = 0$. Physically, this is equivalent to assuming that at $a = 0$ there is an infinite potential barrier (in the same way as in non-relativistic one-dimensional barrier problems), and then the existence of a solution at any 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 values in $\mathbb{R}$, in particular, 0 or negative values. We can conclude that if we want to work in the Heisenberg picture, we must introduce some kind of potential barriers that can prevent the effective scalar factor from taking negative values.

Once we have obtained a self-adjoint extension we apply the effective formulation (1) to the problem

$$\mathrm{i}\hbar\partial_t\Phi(t) = \frac{\hbar^2}{2\gamma^2 a}\partial_a^2\Phi(t) + \rho_0 a_0^3\Phi(t), \tag{B.5}$$

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

$r = 0$, one can take

$$\Psi(a) \equiv \frac{a^{-1}}{(\sigma\pi)^{1/4}} \, \mathrm{e}^{-\frac{\ln^2(a/\bar{a})}{2\sigma}} \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\ln(a/\bar{a})p^*)},$$
$$p^* = -\sqrt{2\rho_0(a_0\bar{a})^3\gamma^2\,\mathrm{e}^{-\frac{9}{4}\sigma} - \hbar^2\left(\frac{25}{4} + \frac{1}{2\sigma}\right)}. \tag{B.6}$$

For this initial state, the effective scale factor, $a_{\mathrm{eff}}(t) = \langle\hat{a}\rangle_{\Phi(t)},$ grows forever for $t > t^*$ in a 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 $\hat{H} = \frac{\hbar^2}{2\gamma^2 a}\partial_a^2 + \frac{\rho_0 a_0^4}{a}$, and the solutions of the equation $\hat{H}\Phi = \pm\mathrm{i}\rho_0 a_0^3\Phi$ are Airy functions $\Phi_{1,\pm} \equiv A\mathrm{i}(\beta_\pm(a \pm \mathrm{i}a_0))$ and $\Phi_{2,\pm} \equiv B\mathrm{i}(\beta_\pm(a \pm \mathrm{i}a_0))$, where $\beta_\pm \equiv \left(\frac{2\gamma^2\rho_0 a_0^3}{\hbar^2}\right)^{1/3}\mathrm{e}^{\pm\mathrm{i}\pi/6}$. In this case, the dimension of both deficiency subspaces is 1; then as in the dust matter case, $\hat{H}$ has infinitely many self-adjoint extensions parametrized by a unitary 1×1 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

$$\Psi(a) \equiv \frac{a^{-1}}{(\sigma\pi)^{1/4}} \, \mathrm{e}^{-\frac{\ln^2(a/\bar{a})}{2\sigma}} \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\ln(a/\bar{a})p^*)},$$
$$p^* = -\sqrt{2\rho_0\left(a_0^2\bar{a}\right)^2\gamma^2\,\mathrm{e}^{-2\sigma} - \hbar^2\left(\frac{25}{4} + \frac{1}{2\sigma}\right)}. \tag{B.7}$$

The following remark is in order. When the three-dimensional curvature is positive ($k = 1$), the Hamiltonian of the system is $H = -\frac{1}{2\gamma^2 a}p_a^2 + \rho(a)a^3 - \frac{1}{2}\gamma^2 c^2 a$. When $\omega > -1/3$ the Hamiltonian constraint restricts the value of the scalar factor to the interval $(0, A)$ with $A = \left(2\rho_0 a_0^{3(\omega+1)}/(c\gamma)^2\right)^{\frac{1}{3\omega+1}}$, and this tells us that, for the Hilbert space, we must take the space $\mathcal{L}^2\,((0, A), a\,da)$. Now for $\omega \leqslant 1$, $a = 0$ is a regular singular point of the ordinary differential equation $\hat{H}\Phi = z_\pm\Phi$, 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. Then, the self-adjoint extensions are parametrized by a 2×2 unitary matrix, and the most natural boundary condition is to assume that wavefunctions vanish at two boundary points. Physically, this means that the scale factor is confined in a very deep potential well, and we have an oscillating universe whose effective scalar factor never vanishes.

B.1. An analytic solution

We consider the dust matter case ($\omega = 0$), and we use the notation

$$C \equiv \rho_0 a_0^3, \qquad K \equiv \frac{\hbar^2}{2\gamma^2}. \tag{B.8}$$

We take the part of the spectrum, with the eigenvalue E, of the Hamiltonian operator which satisfies $C - E > 0$. Then using formula 9.15.1 of [34], one obtains the following eigenfunction: $\phi_E(a) = \sqrt{a}J_{\frac{1}{3}}\left(\frac{2}{3\sqrt{K}}\sqrt{C - E}a^{3/2}\right)$, where $J_{\frac{1}{3}}$ denotes the Bessel function of the first kind.

A solution of the Schrödinger equation is given by

$$\Phi(a,t) = B\int_{-\infty}^{C} \mathrm{d}E\, \mathrm{e}^{-\mathrm{i}\frac{Et}{\hbar}} F(E)\phi_E(a), \tag{B.9}$$

where B is a normalization constant. To obtain an analytic expression for the wavefunction we choose, in the same way as in [9], $F(E) \equiv \frac{1}{2}(C-E)^{1/6}\,\mathrm{e}^{-\frac{C-E}{\delta}}$, where ν and δ are some real, positive constants. Making the change of the variable $r^2 \equiv C - E$ and using equation 11.4.29 of [34], one gets

$$\Phi(a,t) = \frac{B}{2.3^{1/3}.K^{1/6}}a\left(\frac{1}{\delta} - \mathrm{i}\frac{t}{\hbar}\right)^{-4/3} \mathrm{e}^{-\frac{a^3}{9K(\frac{1}{\delta}-\mathrm{i}\frac{t}{\hbar})}}\,\mathrm{e}^{-\mathrm{i}\frac{Ct}{\hbar}}. \tag{B.10}$$

Now we impose the normalization of the wavefunction, i.e. $\|\Phi(0)\| = 1$, to obtain the relation

$$\frac{3K}{2^{10/3}}\delta^{4/3}|B|^2\Gamma(4/3) = 1, \tag{B.11}$$

where Γ denotes Euler's gamma function. Finally, we have to impose $\langle\hat{H}\rangle_{\Phi(0)} = 0$, and thus get

$$\frac{3}{16}\frac{\delta^{7/3}}{2^{1/3}}|B|^2\Gamma(1/3) = C/K. \tag{B.12}$$

Solving these two equations one has that $\delta = \frac{2C}{3}$; that is, we have obtained a solution of our effective formulation given by (B.10). With this solution it is easy to obtain

$$a_{\mathrm{eff}}(t) = \left(\frac{9K\delta}{2}\right)^{1/3}\left(\frac{1}{\delta^2} + \frac{t^2}{\hbar^2}\right)^{1/3}\frac{\Gamma(5/3)}{\Gamma(4/3)}, \tag{B.13}$$

which shows that, for large values of $|t|$, the behavior is $a_{\mathrm{eff}}(t) \propto t^{2/3}$, as in the classical case, and it also shows that the universe bounces at $t = 0$ with a scale factor $a_{\mathrm{eff}}(0) \propto l_p\big(\frac{m_p c^2}{\rho_0 a_0^3}\big)^{1/3}$, m_p being the Planck mass. Finally, the average of the energy density is given by

$$\langle\hat{\rho}\rangle_{\Phi(t)} = K^{-1}\left(\frac{1}{\delta^2} + \frac{t^2}{\hbar^2}\right)^{-1}. \tag{B.14}$$

Appendix C. QFT in curved spacetime 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

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

with $\mathcal{L}_\phi = \frac{1}{2\hbar c^3}\dot{\phi}^2 - \frac{1}{2\hbar c a^2}(\nabla\phi)^2 - \frac{m^2 c}{2\hbar^3}\phi^2 - \frac{1}{12\hbar c^3}R^2\phi^2$, where $R = \frac{6}{a^2}(\dot{a}^2 + a\ddot{a})$ is the scalar curvature. (Note that in this appendix ϕ has dimensions of energy.) Integrating with respect to $\vec{x}$ and expanding ϕ as a Fourier series $\big(\phi = \sum_{\vec{k}\in\mathbb{Z}^3}\phi_{\vec{k}}\,\mathrm{e}^{2\pi\mathrm{i}\frac{\vec{k}.\vec{x}}{L}}\big)$, one obtains $S = \int_{\mathbb{R}} L(t)\,\mathrm{d}t$, with

$$L(t) = L^3\left[-\frac{\gamma^2}{2}\dot{a}^2 a - \rho_0\,(a/a_0)^{-3(\omega+1)}\,a^3 + a^3\sum_{\vec{k}\in\mathbb{Z}^3}\mathcal{L}_{\phi_{\vec{k}}}\right], \tag{C.2}$$

where $\mathcal{L}_{\phi_{\vec{k}}} = \frac{1}{2\hbar c^3}\dot{\phi}_{\vec{k}}^2 - \frac{1}{2\hbar ca^2}\frac{4\pi^2|\vec{k}|^2}{L^2}\phi_{\vec{k}}^2 - \frac{m^2c}{2\hbar^3}\phi_{\vec{k}}^2 - \frac{1}{12\hbar c^3}R^2\phi_{\vec{k}}^2$. Using the conformal time $\mathrm{d}\eta \equiv \frac{ct_p}{a}\,\mathrm{d}t$ (t_p being the Planck time) and defining the function $\psi_{\vec{k}} = \sqrt{\frac{4\pi t_p}{3\hbar}}\frac{a}{c}\phi_{\vec{k}}$, we obtain $L(t)\,\mathrm{d}t \equiv \frac{3L^3}{4\pi}\widetilde{L}(\eta)\,\mathrm{d}\eta$, with

$$\widetilde{L}(\eta) = -\frac{\hbar}{2t_p}\left(\frac{a'}{c}\right)^2 - \widetilde{\rho}_0\,(a/a_0)^{-3(\omega+1)}\frac{a^4}{l_p} + \frac{1}{2}\sum_{\vec{k}\in\mathbb{Z}^3}\left((\psi')_{\vec{k}}^2 - \frac{1}{t_p^2}\left[\frac{4\pi^2|\vec{k}|^2}{L^2} + \left(\frac{a}{l_c}\right)^2\right]\psi_{\vec{k}}^2\right), \tag{C.3}$$

where we have introduced the Compton wavelength $l_c \equiv \frac{\hbar}{mc}$ and defined $\widetilde{\rho}_0 = \frac{4\pi}{3}\rho_0$. Note that in this Lagrangian we have suppressed the terms $-\frac{3}{8\pi}\left(\frac{a'}{a}\psi_{\vec{k}}^2\right)'$.

The conjugate momenta are $p_a = -\frac{\hbar}{l_p}\frac{a'}{c}$, $p_{\psi_{\vec{k}}} = \psi_{\vec{k}}'$, and the Hamiltonian is given by

$$\widetilde{H}(\eta) = -\frac{1}{2m_p}p_a^2 + U(a) + \frac{1}{2}\sum_{\vec{k}\in\mathbb{Z}^3}\left(p_{\psi_{\vec{k}}}^2 + \omega_{\vec{k}}^2(a)\psi_{\vec{k}}^2\right), \tag{C.4}$$

where m_p is the Planck mass, and

$$U(a) \equiv \widetilde{\rho}_0\,(a/a_0)^{-3(\omega+1)}\frac{a^4}{l_p}, \qquad \omega_{\vec{k}}^2(a) \equiv \frac{1}{t_p^2}\left[\frac{4\pi^2|\vec{k}|^2}{L^2} + \left(\frac{a}{l_c}\right)^2\right]. \tag{C.5}$$

The quantum theory is obtained by doing the replacement $p_a \longrightarrow -\mathrm{i}\hbar\partial_a$ and $p_{\psi_{\vec{k}}} \longrightarrow -\mathrm{i}\hbar\partial_{\psi_{\vec{k}}}$. Then, the quantum Hamiltonian is given by

$$\hat{\widetilde{H}} = \frac{\hbar^2}{2m_p}\partial_{a^2}^2 + U(a) + \hat{H}_m(a,\psi), \tag{C.6}$$

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

$$\hat{A}_{\vec{k}}^\dagger \equiv \frac{1}{\sqrt{2\hbar\omega_{\vec{k}}}}\left(-\hbar\partial_{\psi_{\vec{k}}} + \omega_{\vec{k}}\psi_{\vec{k}}\right), \qquad \hat{A}_{\vec{k}} \equiv \frac{1}{\sqrt{2\hbar\omega_{\vec{k}}}}\left(\hbar\partial_{\psi_{\vec{k}}} + \omega_{\vec{k}}\psi_{\vec{k}}\right). \tag{C.7}$$

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

$$\left[\frac{\hbar^2}{2m_p}\partial_{a^2}^2\Psi + U(a)\Psi\right]\chi + \Psi\frac{\hbar^2}{2m_p}\partial_{a^2}^2\chi + \frac{\hbar^2}{m_p}\partial_a\Psi\partial_a\chi + \Psi\hat{H}_m\chi = 0. \tag{C.8}$$

We assume that Ψ is the solution of the equation

$$-\frac{\hbar^2}{2m_p}\partial_{a^2}^2\Psi - U(a)\Psi = 0, \tag{C.9}$$

and we make the change $\Psi = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}S}$; then we obtain the system

$$\begin{cases} \dfrac{(\partial_a S)^2}{2m_p} - U(a) + \dfrac{\mathrm{i}\hbar}{2m_p}\partial_{a^2}^2 S = 0 \\ \dfrac{\hbar^2}{2m_p}\partial_{a^2}^2\chi - \mathrm{i}\hbar\dfrac{\partial_a S}{m_p}\partial_a\chi + \hat{H}_m\chi = 0. \end{cases} \tag{C.10}$$

To solve this set of equations, we neglect (following Rubakov [36]) the second derivative with respect to a. Then we obtain the new system,

$$\begin{cases} \dfrac{(\partial_a S)^2}{2m_p} - U(a) = 0 \\ -\mathrm{i}\hbar \dfrac{\partial_a S}{m_p}\partial_a \chi + \hat{H}_m \chi = 0. \end{cases} \tag{C.11}$$

The first equation is the classical Hamilton–Jacobi equation, and the second one is the quantum Schrödinger equation that can be solved choosing as the solution of the Hamilton–Jacobi equation $S(a) = \int_0^a \sqrt{2m_p U(a)}\,\mathrm{d}a$, and introducing the conformal time $\frac{\mathrm{d}a}{\mathrm{d}\tau} \equiv \frac{\partial_a S}{m_p}$. Then the Schrödinger equation becomes $\mathrm{i}\hbar\partial_\tau \chi = \hat{H}_m(a(\tau), \psi)\chi$.

Finally, we illustrate the procedure to obtain the QFT in curved spacetime from the effective equation $\mathrm{i}\hbar\partial_\eta \Phi = \hat{\hat{H}}\Phi$. Assuming that the matter field is a small perturbation, we look for the solutions of the form $\Phi(a, \psi; \eta) = \Psi(a; \eta)\chi(\psi; \eta)$, where Ψ is the solution of the equation

$$\mathrm{i}\hbar\partial_\eta \Psi = \frac{\hbar^2}{2m_p}\partial^2_{a^2}\Psi + U(a)\Psi, \tag{C.12}$$

and we assume that Ψ is a function concentrated around a classical solution, namely $a_c(\eta)$, of the equation

$$-\frac{1}{2m_p} p_a^2 + U(a) = 0. \tag{C.13}$$

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

We end with a last, interesting remark, namely from the effective formulation, that it is not difficult to obtain the semi-classical Einstein equations. In fact, starting with the condition $\langle\hat{\hat{H}}\rangle_\Phi = 0$, if we take the wavefunction above (now picked around $a_c + \delta a_c$), one approximately obtains

$$-\frac{1}{2m_p} p^2_{a_c+\delta a_c} + U(a_c + \delta a_c) + \langle \hat{H}_m(a_c(\eta) + \delta a_c(\eta), \psi)\rangle_{\chi,\mathrm{ren}} = 0, \tag{C.14}$$

where the quantity $\langle \hat{H}_m(a_c(\eta) + \delta a_c(\eta), \psi)\rangle_\chi$ has been renormalized. Since a_c is the solution of equation (C.13), one also obtains, in the linear approximation, the following back-reaction equation:

$$-\frac{\hbar}{cl_p} a'_c(\delta a_c)' + U'(a_c)\delta a_c + \langle \hat{H}_m(a_c(\eta), \psi)\rangle_{\chi,\mathrm{ren}} = 0. \tag{C.15}$$

Finally, observe that the derivation of the semi-classical Einstein equation from the WDW one is not a completely clear case (see, e.g., [37]).

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