Quantum fate of singularities in a dark-energy dominated universe

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Classical models for dark energy can exhibit a variety of singularities, many of which occur for scale factors much bigger than the Planck length. We address here the issue of whether some of these singularities, the big freeze and the big *démarrage*, can be avoided in quantum cosmology. We use the framework of quantum geometrodynamics. We restrict our attention to a class of models whose matter content can be described by a generalized Chaplygin gas and be represented by a scalar field with an appropriate potential. Employing the DeWitt criterion that the wave function be zero at the classical singularity, we show that a class of solutions to the Wheeler-DeWitt equation fulfilling this condition can be found. These solutions thus avoid the classical singularity. We discuss the reasons for the remaining ambiguity in fixing the solution.

I. INTRODUCTION

Understanding the observed acceleration of the Universe may affect our understanding of gravity as well as enlarge the framework of particle physics; see, for example, [1–4] for some reviews on the state of the art. The presence of precision observations is particularly promising in this respect [5].

Even though a cosmological constant is the simplest way to explain phenomenologically the late-time acceleration of our Universe, it is not entirely appealing from a theoretical point of view. The reason is the mismatch between the required observational value and the expected one from theoretical grounds [6]. This has induced a whole manufacture of theoretical model building, aiming at an explanation of the recent speedup of the Universe. Most of these models invoke a dark-energy component with negative pressure [7] or a modification of gravity on a large scale [8] which, by weakening the gravitational interaction, achieve the accelerated expansion. More exotic explanations invoke ideas of a multiverse and may therefore have to use the anthropic principle or isotropic and inhomogeneous cosmologies which violate the cosmological principle [9–11].

In practical applications and for a homogeneous and isotropic universe, which is a good approximation for our Universe on large scales, whatever the entity responsible for the recent acceleration may be, it can be described effectively through an equation of state parameter w. This parameter w is just the ratio between the pressure and the energy density of the unknown entity (sometimes designated as "dark energy") and may, of course, be time-dependent. The value of w is observationally very close to $w = -1$, that is, the equation of state for a cosmological constant. However, if w is larger or smaller than $w = -1$, the future of the Universe will be dramatically different. Let us mention that indications of a decaying dark energy have recently been reported [12].

Our main interest here lies not so much in the observational significance of such models but in their relevance for understanding the quantization of gravity. The search for a consistent theory of quantum gravity is among the main open problems in theoretical physics [13]. One aspect is the fate of the singularities which are prevalent in the classical theory of general relativity. The hope is that a consistent quantum theory of gravity is free of such singularities. This aspect can most easily be investigated in the framework of quantum cosmology: the application of quantum theory to the Universe as a whole [13,14]. Because of our restriction to homogeneous models, the corresponding framework of quantum cosmology does not encounter the mathematical problems of the full theory. We also emphasize that quantum cosmology is a nonperturbative framework and thus different from approaches employing "quantum corrections" to the classical theory.[1] Within this context, some of the dark-energy models are particularly suitable. Furthermore, if one of the models applies to our real Universe, this would provide us with important insights into its past and future, which could be a singularity-free and timeless quantum world.

Indeed, during the past years, it has been shown that some dark-energy scenarios with $w < -1$, dubbed phantom energy models [17], can induce a new type of singu-

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[1]For reviews on cosmological singularities and string theory, cf. [15,16], and references therein.

larity called the big-rip singularity. This is a singularity where both density and pressure diverge and which is attained for a universe that expands to infinity in a finite time. The quantum version of such a situation was extensively investigated in [18] (see also [19,20]). It was found there that the semiclassical approximation necessarily breaks down for large-enough scale factors, and so the singularity theorems no longer apply.

It was soon realized that the big-rip singularity is not the unique singularity related to dark energy and that different types of singularities could show up [21–23]. One of them is the big-brake singularity, which is obtained for a universe in the future and which is characterized by an infinite deceleration; the universe comes to an abrupt halt. The quantum cosmology of such a model was discussed at length in [24]. It was found there that, given reasonable assumptions, the wave function vanishes in the region of the classical singularity, which we can safely interpret as singularity avoidance. From theoretical investigations such classical singularities are well known [25], but in the context here they occur within models possessing observational relevance.

In this work we are interested in the generalization of these quantum-cosmological results to a broader class of models. We shall find that the singularity avoidance is there effective, too. We are mainly concerned with two types of singularities known as the big-freeze[2] and big-*démarrage* singularity, respectively [29]. Let us give a brief characterization of them:

(i) The big-freeze singularity (or type-III singularity in the nomenclature of [22]) takes place at a finite scale factor and finite cosmic time in a (flat) Friedmann-Lemaître-Robertson-Walker (FLRW) universe. At this singularity, both the Hubble rate and its cosmic derivative blow up. (This is not the case for a big-brake singularity.) Such a singularity can be induced by a generalized Chaplygin gas (GCG) [29]. The GCG is a perfect fluid which satisfies the following polytropic equation of state [30]:

$$p = -\frac{A}{\rho^{\beta}}, \qquad (1)$$

where A and β are constants. This equation of state was introduced in cosmology with the intention to unify the dark sectors of the Universe, that is, dark matter and dark energy [30]. How this is achieved

can be seen from the conservation of the energy-momentum tensor of such a fluid in a homogeneous and isotropic universe. It implies

$$\rho = \left(A + \frac{B}{a^{3(1+\beta)}}\right)^{1/(1+\beta)}, \qquad (2)$$

where B is a constant. Therefore, if A, B, and $1 + \beta$ are positive, the energy density ρ interpolates between a dust energy density for a small scale factor and a constant energy density for a large scale factor. However, it is possible that the GCG can exclusively correspond to dark energy in a FLRW universe. The behavior of a GCG can be quite different if the parameters A, B, and $1 + \beta$ are not all positive. In particular, it can induce different sorts of singularities [31]. Moreover, it was shown that a phantom GCG, that is, a fluid which satisfies the polytropic equation of state (1) for $\rho > 0$ and $p + \rho < 0$, can induce a future big-freeze singularity [29]. It was also realized that even a GCG fulfilling the null, strong, and weak energy conditions can lead to a big-freeze singularity [31] in the past.

(ii) In Ref. [31], it was also shown that a sudden singularity (or type-II singularity in the nomenclature of [22]) can be induced by a GCG. A sudden singularity is characterized by the fact that the Hubble rate is finite, while its cosmic derivative blows up at a finite scale factor. If the GCG fulfils the null, strong, and weak energy conditions, then the sudden singularity corresponds to a big-brake singularity [24] which takes place in the future when the universal expansion is stopped by an infinite deceleration. On the other hand, if the GCG corresponds to a phantom fluid, the sudden singularity takes place in the past. In analogy with the terminology of the big-brake singularity, we call this kind of sudden singularity a big-*démarrage* singularity because the universe starts its expansion with an infinite acceleration. Since the big-brake singularity has been studied in [24], we shall restrict our attention here to the phantom model exhibiting a big-*démarrage* singularity.

An interesting feature of these singularities is the fact that they can occur in a macroscopic universe, that is, for large values of the scale factor. A pertinent question is then whether quantum gravitational effects can resolve these singularities. Would that mean that there could be quantum effects in the macroscopic universe? *How* could we expect these singularities to be resolved through quantum gravity? This is the major motivation standing behind the quantum analysis of the big-freeze and big-*démarrage* singularities. We shall carry out our quantization in the geometrodynamical framework, using the three-metric and its conjugate momentum as fundamental variables. The governing equation in this framework is the Wheeler-DeWitt equation. One can invoke various reasons why this framework is

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[2]It has been recently shown that a big-freeze singularity might be simply an indication that a brane is about to change from a Lorentzian to a Euclidean signature [26], even though the brane and the bulk remain fully regular everywhere. This kind of behavior can happen in some braneworld models where the bulk is always Lorentzian and does not change its signature. If the brane and the bulk change simultaneously their signature like in the models discussed in [27,28], observers at the brane would not perceive to go into such a big-freeze singularity.

appropriate for studying the question at hand[3] [37]. Perhaps the most compelling one is the fact that the Wheeler-DeWitt equation is the wave equation which straightforwardly leads to the Einstein equations in the semiclassical limit.

Our paper is organized as follows. In Sec. II, we review the classical cosmology with a generalized Chaplygin gas leading to a past/future big-freeze singularity or a past sudden singularity. To be able to study the quantum behavior, the GCG has to be mimicked by a fundamental field because also the matter part should have its own degrees of freedom. The representation of the GCG in terms of minimally coupled scalar fields will be given in Sec. III. The remainder of this article is concerned with the quantum properties of these scenarios. In Sec. IV, we obtain solutions for the quantum-cosmological model with phantom and nonphantom GCG evolving to and from a big-freeze singularity, respectively. We investigate whether this singularity can be quantum gravitationally avoided. The big-*démarrage* singularity is also addressed at the quantum-cosmological level. The (general) results are then discussed for different types of boundary conditions in Sec. V. We present explicit results for the quantum states that avoid the singularities and discuss further consequences. Section VI gives our conclusions and outlook. In the appendix, we present a justification of the gravitational wave function approximation used in the paper.

II. THE CLASSICAL BIG-FREEZE AND BIG-DÉMARRAGE SINGULARITIES INDUCED BY A GENERALIZED CHAPLYGIN GAS

A. The big-freeze singularity without phantom matter

We review here a particular case of the plain generalized Chaplygin gas [31], that is, a fluid which satisfies the polytropic equation of state (1) and fulfils the null, strong, and weak energy conditions. Such an equation of state may induce a big-freeze singularity in the past. This is the case[4] when $A < 0$, $B > 0$, and $1 + \beta < 0$. Then the energy density can be written as

$$\rho = |A|^{1/(1+\beta)} \left[-1 + \left(\frac{a_{\min}}{a} \right)^{3(1+\beta)} \right]^{1/(1+\beta)}, \quad (3)$$

where

$$a_{\min} = \left| \frac{B}{A} \right|^{1/3(1+\beta)} \quad (4)$$

denotes the minimal scale factor, which is the value where the singularity occurs. We consider a spatially flat homo-

geneous and isotropic universe filled with this sort of fluid. Then, at the minimum scale factor $a_{\min}$, the energy density blows up and so does the Hubble rate. Similarly the pressure, which reads

$$p = |A|^{1/(1+\beta)} \left[-1 + \left(\frac{a_{\min}}{a} \right)^{3(1+\beta)} \right]^{-\beta/(1+\beta)}, \quad (5)$$

diverges when the scale factor approaches its minimum value $a_{\min}$. Notice that the pressure is positive, and therefore a FLRW universe filled with this fluid would never accelerate. This particular choice of parameters can thus not describe the acceleration of the current Universe. In fact, the deceleration parameter

$$q = \tfrac{1}{2}(1 + 3w) \quad (6)$$

is always positive. Figure 1 displays $w = p/\rho$. On the other hand, the Raychaudhuri equation implies that at $a_{\min}$ the cosmic-time derivative of the Hubble rate also diverges. In order to show that the event that takes place at $a_{\min}$ corresponds to a past big-freeze singularity, it remains to be proven that from a given finite scale factor the cosmic time elapsed since the singularity took place is finite. This can be done by integrating the Friedmann equation. The cosmic time in terms of the scale factor reads [31]
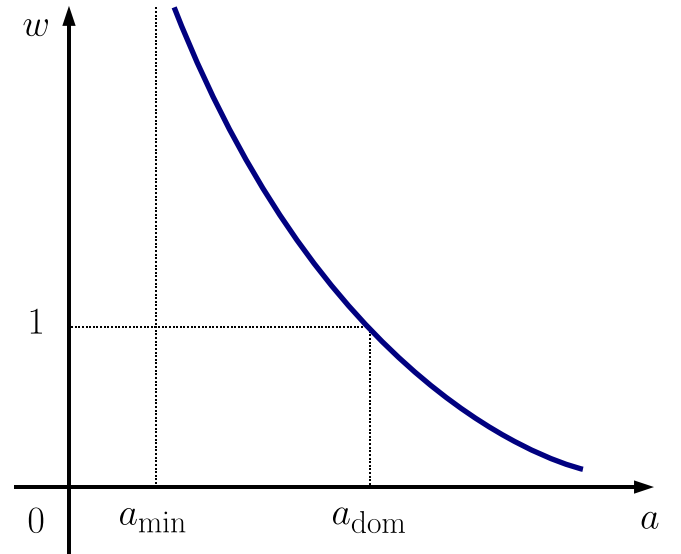

FIG. 1 (color online). Plot of the ratio of pressure and energy density w for the generalized Chaplygin gas analyzed in this section as a function of the scale factor [31]. The dominant energy condition is not fulfilled for a scale factor smaller than a_{dom}.

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[3]For a discussion on singularity avoidance within loop quantum cosmology, cf. [32]; for an earlier discussion where geometrodynamical elements were present, cf. [33–36].

[4]The conclusion reached in this section also holds for $A > 0$, $B < 0$, $1 + \beta < 0$, and $1 + \beta = 1/(2n)$, with n some negative integer number. For simplicity, we shall disregard this case.

$$t - t_{\min} = -\frac{2}{\kappa\sqrt{3}} \frac{|A|^{-1/2(1+\beta)}}{1+2\beta}$$
$$\times \left[\left(\frac{a_{\min}}{a}\right)^{3(1+\beta)} - 1\right]^{(1+2\beta)/2(1+\beta)} \left(\frac{a}{a_{\min}}\right)^{3(1+\beta)}$$
$$\times F\left(1, 1; \frac{3+4\beta}{2(1+\beta)}; 1 - \left(\frac{a}{a_{\min}}\right)^{3(1+\beta)}\right), \quad (7)$$

where $\kappa^2 = 8\pi G$ and $F(b, c; d; e)$ is a hypergeometric function; see, for example, [38]. In the previous expression, $t_{\min}$ corresponds to the cosmic time when a universe filled by this sort of generalized Chaplygin gas would emerge from a past big-freeze singularity at $a = a_{\min}$. We thus find here a singularity at finite scale factor $a_{\min}$ and finite cosmic time $t_{\min}$, where both energy density and pressure blow up, as the Hubble parameter and its cosmic derivative do as well. It can easily be checked that the cosmic time elapsed since the universe emerged from the past big-freeze singularity until it has a given size (at a given t) is finite,[5] that is, $t - t_{\min}$ is bounded for any finite scale factor. Before concluding this section, we notice that, although the generalized Chaplygin gas analyzed here fulfils the null, strong, and weak energy conditions, it violates the dominant energy condition for scale factors smaller than a_{dom}, where

$$a_{\mathrm{dom}} = 2^{-1/3(1+\beta)} a_{\min}. \quad (8)$$

At a_{dom} the pressure equals the energy density and for smaller scale factors $\rho < p$. This situation is schematically shown in Fig. 1.

B. The big-freeze singularity with a phantom GCG

The big-freeze singularity discussed above may also take place in the future at a scale factor $a = a_{\max}$. This is possible if the GCG exhibits a phantom behavior, that is, if it satisfies $p + \rho < 0$ [39]. Eventually, the pressure will be so negative that the universe not only accelerates but is even superaccelerating; that is, the Hubble rate grows as the universe expands. This is certainly a model capable of describing dark energy. When the scale factor approaches $a_{\max}$, the energy density as well as the pressure diverge in a finite future cosmic time [31]. This phantom GCG induces a big-freeze singularity, although in this case the event happens in the future instead of, as above, in the past [29,31]. Such a future big-freeze occurs for $A > 0$, $B < 0$, and $1 + \beta < 0$. Being more precise, the energy density in this case reads

$$\rho = A^{1/(1+\beta)}\left[1 - \left(\frac{a_{\max}}{a}\right)^{3(1+\beta)}\right]^{1/(1+\beta)}, \quad (9)$$

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[5]A hypergeometric series $F(b, c; d; e)$, also called a hypergeometric function, converges at any value e such that $|e| \leq 1$ whenever $b + c - d < 0$. However, if $0 \leq b + c - d < 1$, the series does not converge at $e = 1$. In addition, if $1 \leq b + c - d$, the hypergeometric function blows up at $|e| = 1$ [38].

while the pressure is

$$p = -A^{1/(1+\beta)}\left[1 - \left(\frac{a_{\max}}{a}\right)^{3(1+\beta)}\right]^{-\beta/(1+\beta)}, \quad (10)$$

where

$$a_{\max} = \left|\frac{B}{A}\right|^{1/3(1+\beta)} \quad (11)$$

is the maximal value of the scale factor.

C. The big-*démarrage* singularity with a phantom GCG

The GCG is also known to induce future or past sudden singularities [24,31,40]. The following cases can be distinguished:

(1) If the GCG fulfils the null, strong, and weak energy conditions with $A < 0$, $B > 0$, and $\beta > 0$, a universe filled with this sort of gas would face a future sudden singularity, which is just the big-brake singularity already mentioned above. For $\beta = 1$ this fluid was named an anti-Chaplygin gas in [24] because the case with $\beta = 1$ and $A > 0$ is usually called the Chaplygin case. Since this model was discussed at length in [24], we shall disregard it here.

(2) If the GCG is a phantom fluid with $A > 0$, $B < 0$, and $\beta > 0$, a universe filled with this fluid would face a past sudden singularity; that is, the classical evolution starts at a finite scale factor and energy density while the pressure of the fluid diverges. We name this past sudden singularity a big-*démarrage* singularity as the universe would start its classical evolution with an extremely large acceleration due to the very negative pressure of the fluid. This phantom GCG corresponds to an example where a future big-rip singularity can be avoided even for phantom matter [39] as in this case the universe would asymptotically approach de Sitter space in the future. Here we are rather interested in the early behavior of a universe close to the big-*démarrage* singularity.

Let us add a few more comments on the second case stated above. The energy density and pressure of the phantom GCG can be expressed as in (9) and (10) after substituting $a_{\max}$ by $a_{\min}$ where the initial scale factor $a_{\min}$ can be expressed as in (4). The phantom nature of this fluid induces a superacceleration of the universe which, in particular, implies that a universe filled with this fluid would be accelerating.

III. THE CLASSICAL BIG-FREEZE AND BIG-*DÉMARRAGE* SINGULARITIES INDUCED BY SCALAR FIELDS

A perfect fluid is an effective description of matter. As such it is valid only on certain (large) scales. At the quantum level, we may need a more fundamental descrip-

tion of matter. We herein choose the simplest possible one: a minimally coupled scalar field. In the following subsections, we formulate the standard and phantom GCG in terms of standard and phantom scalar fields, respectively. This step is an important preparation for the quantum part because the wave function is defined on configurations space; that is, it will depend on the scale factor and the scalar field.

A. The big-freeze singularity driven by a standard canonical scalar field

We first show how the GCG given in Sec. II A can be described by a standard minimally coupled scalar field whose energy density and pressure in a homogeneous and isotropic universe read, respectively,

$$\rho_\phi = \tfrac{1}{2}\dot{\phi}^2 + V(\phi), \qquad p_\phi = \tfrac{1}{2}\dot{\phi}^2 - V(\phi). \qquad (12)$$

The dot corresponds to the derivative with respect to cosmic time. Then by imposing that ρ_ϕ and p_ϕ satisfy the equation of state (1), the kinetic energy density and the scalar-field potential evolve with the scale factor as

$$\dot{\phi}^2 = |A|^{1/(1+\beta)} \frac{(\frac{a_{\min}}{a})^{3(1+\beta)}}{[(\frac{a_{\min}}{a})^{3(1+\beta)} - 1]^{\beta/(1+\beta)}},$$

$$V(a) = \frac{1}{2}|A|^{1/(1+\beta)} \frac{(\frac{a_{\min}}{a})^{3(1+\beta)} - 2}{[(\frac{a_{\min}}{a})^{3(1+\beta)} - 1]^{\beta/(1+\beta)}}. \qquad (13)$$

Therefore, the scalar field changes with the scale factor as (cf. Fig. 2)

$$|\phi - \phi_{\min}|(a) = \frac{2\sqrt{3}}{3\kappa|1+\beta|} \ln\left[\left(\frac{a_{\min}}{a}\right)^{(3/2)(1+\beta)} + \sqrt{\left(\frac{a_{\min}}{a}\right)^{3(1+\beta)} - 1}\right], \qquad (14)$$
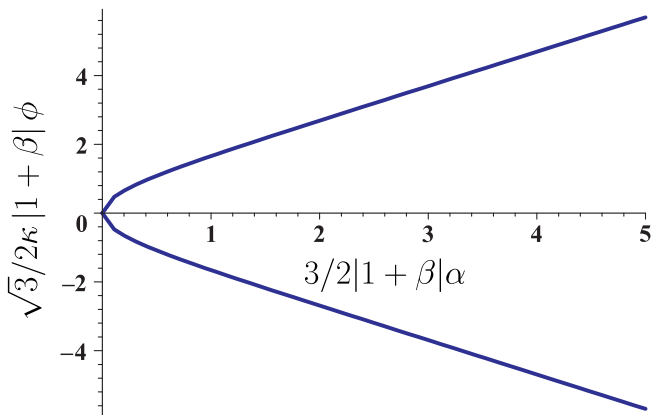

FIG. 2 (color online).   Plot of the scalar field versus the logarithmic scale factor $\alpha = \ln(a/a_0)$, where a_0 corresponds to the location of the singularity in the respective models. This plot corresponds to a past big-freeze singularity where $a_0 = a_{\min}$ [see Eq. (14)].
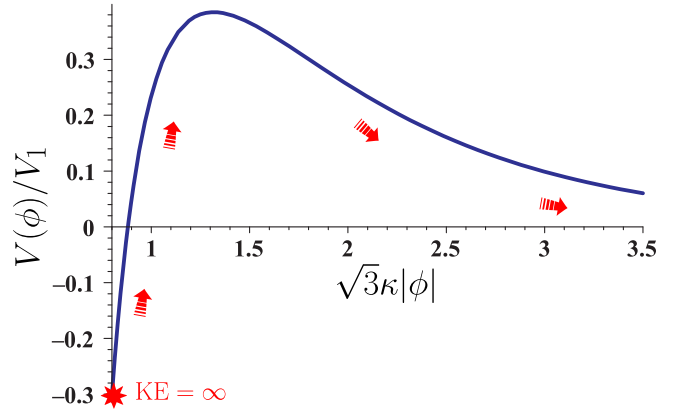

FIG. 3 (color online).   Plot of the potential (15) as a function of the scalar field for the value $\beta = -3$. The star denotes the location of the singularity, KE denotes the kinetic energy of the scalar field, and the arrows denote the trajectory of the scalar field.

where $\phi_{\min}$ corresponds to the value of the scalar field at $a_{\min}$, where the singularity occurs; we shall set $\phi_{\min} = 0$ for simplicity. Finally, by combining (13) and (14), the scalar-field potential reads

$$V(\phi) = V_1\left[\sinh^{2/(1+\beta)}\left(\frac{\sqrt{3}}{2}\kappa|1+\beta||\phi|\right) - \frac{1}{\sinh^{2\beta/(1+\beta)}(\frac{\sqrt{3}}{2}\kappa|1+\beta||\phi|)}\right], \qquad (15)$$

where $V_1 = |A|^{1/(1+\beta)}/2$. Notice that at the minimum scale factor or at $\phi = 0$ the potential is negative and divergent. In fact, the potential can be approximated in this region by[6]

$$V(\phi) \simeq -V_1\left(\frac{\sqrt{3}}{2}\kappa|1+\beta||\phi|\right)^{-2\beta/(1+\beta)}. \qquad (16)$$

We recall that $1 + \beta < 0$ and therefore $-2\beta/(1+\beta) < -2$; that is, $V(\phi)$ is at the big-freeze singularity more singular than an inverse-square potential. This is crucial for the discussion of the quantum theory below. On the other hand, for large values of the scale factor or at large values of the scalar field, we have

$$V(\phi) \simeq 2^{-2/(1+\beta)} V_1 \exp(-\sqrt{3}\kappa|\phi|). \qquad (17)$$

The general behavior of the potential is shown in Fig. 3. The scalar field starts with an infinite kinetic energy (at the past big-freeze singularity) climbing up the potential until it reaches its top and then starts rolling down the potential hill. When the potential vanishes, the scale factor is equal to a_{dom}. Hence, the dominant energy density is violated

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[6]At the lowest order, the first term in (15) does not contribute to the approximation made in (16) because $-2\beta/(1+\beta) < 2/(1+\beta) < 0$.

when the scalar field takes a value such that the potential becomes negative.

B. The big-freeze singularity driven by a phantom scalar field

Similarly to the case just considered, the GCG discussed in Sec. II B can also be described by a minimally coupled scalar field, although in this case the phantom nature of the GCG implies that the scalar field does not have the standard kinetic term; therefore, its energy density and pressure read, respectively,

$$\rho_\phi = -\tfrac{1}{2}\dot{\phi}^2 + V(\phi), \qquad p_\phi = -\tfrac{1}{2}\dot{\phi}^2 - V(\phi) \quad (18)$$

for a FLRW universe. Equating the previous quantities to (9) and (10), we obtain

$$\dot{\phi}^2 = A^{1/(1+\beta)} \frac{(\frac{a_{\max}}{a})^{3(1+\beta)}}{[1 - (\frac{a_{\max}}{a})^{3(1+\beta)}]^{\beta/(1+\beta)}},$$

$$V(a) = \frac{1}{2} A^{1/(1+\beta)} \frac{2 - (\frac{a_{\max}}{a})^{3(1+\beta)}}{[1 - (\frac{a_{\max}}{a})^{3(1+\beta)}]^{\beta/(1+\beta)}}. \quad (19)$$

Consequently,

$$\phi = \pm \frac{2}{\kappa\sqrt{3}} \frac{1}{1 + \beta} \arccos\left[\left(\frac{a_{\max}}{a}\right)^{3(1+\beta)/2}\right]. \quad (20)$$

In Fig. 4, we show how the scalar field is correlated with the scale factor. From the last equation, one can read off that the scalar field vanishes when the scale factor reaches its maximal classically allowed value. By using the relations (19) and (20) we find the following expression for the potential:
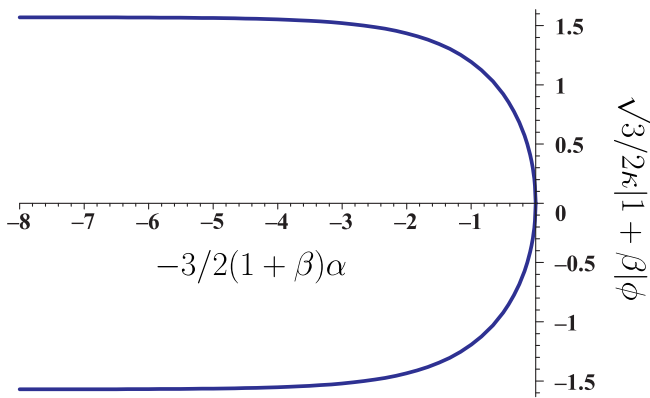

FIG. 4 (color online). Plot of the scalar fields versus the logarithmic scale factor $\alpha = \ln(a/a_0)$, where a_0 corresponds to the location of the singularity in the respective models. The plot corresponds to a future big-freeze/(past)big-*démarrage* singularity [see Eq. (20)]. In the scenario with a future big-freeze or a (past) big-*démarrage* singularity, the quantity $-3/2(1 + \beta)\alpha$ is always negative.
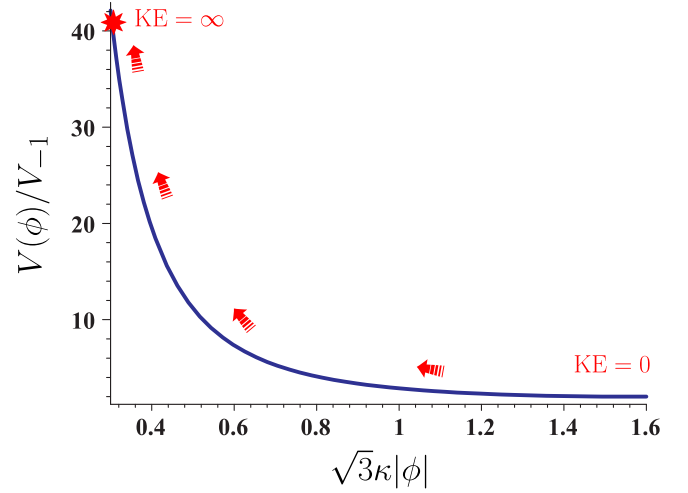

FIG. 5 (color online). Plot of the potential defined in (21) as a function of the scalar field for the value $\beta = -3$. The star denotes the location of the singularity, KE denotes the kinetic energy of the scalar field, and the arrows indicate the trajectory of the scalar field.

$$V(\phi) = V_{-1}\left[\frac{1}{\sin^{2\beta/(1+\beta)}(\frac{\sqrt{3}}{2}\kappa|1 + \beta||\phi|)} + \sin^{2/(1+\beta)}\left(\frac{\sqrt{3}}{2}\kappa|1 + \beta||\phi|\right)\right], \quad (21)$$

where $V_{-1} = A^{1/(1+\beta)}/2$ and $0 < (\sqrt{3}/2)\kappa|1 + \beta||\phi| \leq \pi/2$ (see Fig. 5).

The big-freeze singularity at $a = a_{\max}$ is now located at $\phi = 0$ where the scalar-field potential can be approximated by[7]

$$V(\phi) \simeq V_{-1}\left(\frac{\sqrt{3}}{2}\kappa|1 + \beta||\phi|\right)^{-2\beta/(1+\beta)}. \quad (22)$$

This potential [also the exact potential (21)] can be deduced from the expression (16) [respectively, (15)] by rotating $\phi \rightarrow i\phi$ and taking into account that A changes sign. Notice that this implies that there is a change of sign of the potential (16) after performing such an analytical continuation.

In general, the potential (22) corresponds to a singular potential. However, for large-enough β (and again for $\phi \rightarrow 0$), $V(\phi)$ behaves effectively as an inverse-square potential; that is,

$$V(\phi) \simeq V_{-1}\left(\frac{\sqrt{3}}{2}\kappa|1 + \beta||\phi|\right)^{-2}, \qquad 1 \ll |\beta|. \quad (23)$$

The scalar field starts its cosmological evolution with a vanishing kinetic energy density at $\sqrt{3}/2\kappa|1 + \beta||\phi| = \pi/2$, and then it climbs up through the potential reaching

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[7]Again, the second term in (21) does not contribute to the potential (22) because $-2\beta/(1 + \beta) < 2/(1 + \beta) < 0$.

an infinite kinetic energy when the classical universe reaches its maximum size, that is, when $\phi \to 0$ [see Fig. 5]. This is a usual feature of phantom scalar fields. Notice as well that the standard canonical scalar field with the potential (15) also climbs through its potential, but in this case the reason behind this strange behavior is the initial infinite kinetic energy of the scalar field when $\phi \to 0$.

C. The big-*démarrage* singularity driven by a phantom scalar field

Similarly to the above cases, one can also show that the phantom GCG leading to a big-*démarrage* singularity can be mimicked by a minimally coupled phantom scalar field ϕ, where ϕ and the scalar-field potential $V(\phi)$ are given, respectively, by Eqs. (20) and (21) after substituting $a_{\max}$ by $a_{\min}$; see also Figs. 4 and 6. The expressions given in (19) are also valid after exchanging $a_{\max}$ by $a_{\min}$. The scalar field starts moving away from the singularity (located at $\phi = 0$ or $a = a_{\min}$) by rolling down the potential with an infinite kinetic energy. The phantom nature of the scalar field implies that ϕ loses its kinetic energy as it rolls down the potential; cf. Fig. 6. In fact, when the scalar field reaches the tail of the potential, that is, $\sqrt{3}/2\kappa|1 + \beta||\phi| \to \pi/2$, its kinetic energy is approaching zero, which is in agreement with the asymptotic de Sitter-type behavior of a universe filled by this phantom GCG.

Close to the singularity ($\phi \to 0$), $V(\phi)$ can be approximated by (22). Because $\beta > 0$, this potential does not correspond to a singular potential, although for $1 \ll \beta$ it behaves as an inverse-square potential. Notice as well that for $\beta = 1$ the potential behaves as a Coulomb potential like its nonphantom version [24].
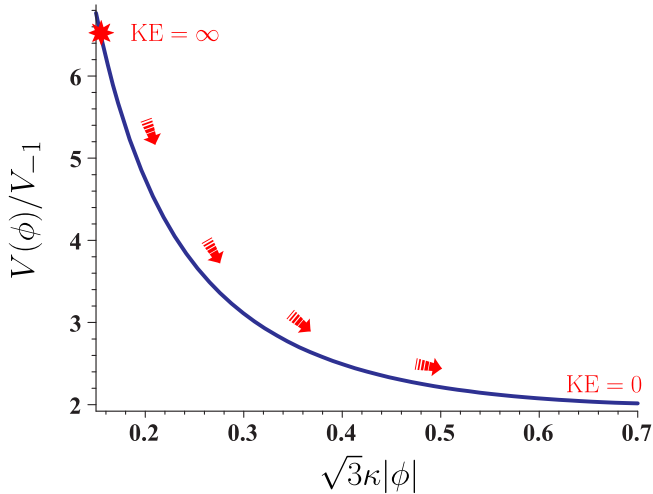

FIG. 6 (color online). Plot of the potential defined in (21) as a function of the scalar field for the value $\beta = 3$. The star denotes the location of the singularity, KE denotes the kinetic energy of the scalar field, and the arrows indicate the trajectory of the scalar field.

IV. WHEELER-DEWITT EQUATION AND QUANTUM STATES

In this section, we shall describe the quantization of the classical scenarios discussed above. This will be carried out in the quantum geometrodynamical framework. Its central equation is the Wheeler-DeWitt equation, depending on the configuration space variables (a, ϕ). From the solutions obtained, we shall retrieve information concerning the above GCG models with regard to their quantum behavior at the classical singularity.[8] A discussion of the influence of different boundary conditions on the wave function is presented in the next section.

Before proceeding to more technical aspects, let us mention that, even though singularity avoidance is a major touchstone for any quantum gravity theory, no consensus regarding the criteria that may account for such an avoidance exists. This is mainly due to the fact that the criteria that one admits depend strongly on how one interprets the wave function of the universe. Divergent opinions on that interpretation arise because quantum gravity is itself a timeless theory [13]. In this respect it differs from any other quantum field theory, and there is not yet any agreement about the appropriate interpretational framework.

One possible line to establish a reasonable research criterion is to regard the quantum-cosmological wave function as the fundamental entity from which our spacetime can be derived in an appropriate limit. The recovery of spacetime can be expected to occur only in special regions of configuration space. The derivation of the semiclassical limit is performed by a Born-Oppenheimer type of approximation scheme with decoherence as an essential ingredient; cf. [13] and the references therein. The gravitational part of the wave function is usually taken to be of a WKB form, which means that narrow wave packets around classical trajectories would not spread. But wave packets which are initially peaked around classical trajectories may not remain so along the entire trajectory. Such a dispersion is unavoidable in a quantum universe whose classical version exhibits recollapse [42]. Thus, a spreading of the wave packet signals a breakdown of the semiclassical approximation; one can then no longer associate with the wave function a classical spacetime as an approximate concept. Such a spreading necessarily occurs when approaching the region of the classical big-rip singularity in quantum phantom cosmology, a phenomenon which we interpreted in [18] as singularity avoidance.

Another sufficient (but by no means necessary) criterion for singularity avoidance is the vanishing of the wave function at the classical singularity; there is then no possibility for such a singularity to occur in any limit. Vanishing of the wave function as a criterion for singularity avoidance was first suggested by DeWitt in his pioneering paper [43].

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[8]The generalized Chaplygin has been previously analyzed from a quantum point of view in different setups (see Ref. [41]).

Singularity avoidance in this sense occurred for the big-brake singularity [24]. Vanishing of the wave function will also be in the present section the appropriate criterion for singularity avoidance.

Let us, then, turn to a detailed analysis of the quantum versions for the above discussed classical models. The wave function satisfies the Wheeler-DeWitt equation, which with the Laplace-Beltrami factor ordering reads

$$\frac{\hbar^2}{2}\left(\frac{\kappa^2}{6}\frac{\partial^2}{\partial\alpha^2} - \ell\frac{\partial^2}{\partial\phi^2}\right)\Psi(\alpha,\phi) + a_0^6 e^{6\alpha}V(\phi)\Psi(\alpha,\phi) = 0, \tag{24}$$

where $V(\phi)$ is given in (15) for the standard scalar-field model and in (21) for both phantom scalar-field models. We have introduced the new variable $\alpha := \ln(\frac{a}{a_0})$ and assume that a_0 corresponds to the location of the singularity in the respective models. In the following, we shall use $\tilde{a} := \frac{a}{a_0}$ instead of a such that $\tilde{a}_0 = 1$ holds. For simplicity, we shall drop the tilde. Recall that $\kappa^2 = 8\pi G$. We have introduced the parameter ℓ in order to distinguish between the phantom and nonphantom scalar fields. For the phantom scalar field we have $\ell = -1$, whereas we have $\ell = 1$ for ordinary scalar-field matter. Note that a fundamental length scale is necessary in the Wheeler-DeWitt equation to yield correct dimensions. To solve this equation, we make the ansatz

$$\Psi(\alpha,\phi) = \varphi_k(\alpha,\phi)C_k(\alpha), \tag{25}$$

where k is *a priori* not restricted to real values. Furthermore, we require φ_k to satisfy

$$-\ell\frac{\hbar^2}{2}\frac{\partial^2\varphi_k}{\partial\phi^2} + a_0^6 e^{6\alpha}V(\phi)\varphi_k = E_k(\alpha)\varphi_k. \tag{26}$$

Such a Born-Oppenheimer type of ansatz was first used in quantum cosmology in [42] in the study of wave packets. It assumes the approximate validity of a quasiseparability between α and ϕ; that is, the matter part φ_k depends only adiabatically on the scale factor. We discuss the validity of the Born-Oppenheimer approximation in the appendix.

As the potentials (15) and (21) are rather complicated, we solve the Wheeler-DeWitt equation for certain ranges of $|\phi|$ and approximate the respective potential there. For the study of singularity avoidance, the region of primary interest is $|\phi| \ll 1$. This corresponds in each model to the vicinity of the singularity. In this region, the potential is approximated by (16) for the ordinary scalar field and by (22) in the case of the phantom field. Introducing the notation

$$V_\alpha := a_0^6 e^{6\alpha}V_\ell\left[\frac{\sqrt{3}\kappa}{2}|1+\beta|\right]^{-2\beta/(1+\beta)}, \tag{27}$$

we find that φ_k has to satisfy

$$-\ell\frac{\hbar^2}{2}\frac{\partial^2\varphi_k}{\partial\phi^2} - \ell V_\alpha|\phi|^{-2\beta/(1+\beta)}\varphi_k = E_k(\alpha)\varphi_k. \tag{28}$$

Defining $k^2 := \frac{2E_k}{\hbar^2}$ and $\tilde{V}_\alpha := \frac{2V_\alpha}{\hbar^2}$, we finally arrive at

$$\varphi_k'' + [\ell k^2 + \tilde{V}_\alpha|\phi|^{-2\beta/(1+\beta)}]\varphi_k = 0, \tag{29}$$

where $'$ denotes a derivative[9] with respect to ϕ. We recognize that this equation is formally the same as the radial part of the stationary Schrödinger equation for an *attractive* potential of inverse power $V \sim r^{-2\beta/(1+\beta)}$, where $|\phi|$ plays the role of the radial coordinate r, and the angular momentum vanishes.

Equation (29) is the central equation for the following discussion. Because it formally resembles the Schrödinger equation, we are able to make use of results encountered in quantum mechanics. Potentials of the type $V \sim r^{-2\beta/(1+\beta)}$ are there called *singular* [44,45]. Any potential that approaches (plus or minus) infinity faster than r^{-2} for $r \to 0$ belongs to this class. For an attractive r^{-2} potential there exists a transitional case: If the coupling is more negative than a critical value, the potential is singular and otherwise regular.

Analytical solutions for polynomial singular potentials are known for the inverse-square, inverse fourth-power, and inverse sixth-power potentials. The inverse-square potential is realized for $|\beta| \gg 1$, where β is chosen such that $|1 + \beta||\phi|$ is still small. The inverse fourth-power potential corresponds to $\beta = -2$, whereas the inverse sixth-power potential is realized for $\beta = -\frac{3}{2}$.

In our paper we shall focus on the case $|\beta| \gg 1$ for the standard scalar field as well as the two phantom field models. We thus deal with the case of the inverse-square potential $\frac{\tilde{V}_\alpha}{|\phi|^2}$ with

$$\tilde{V}_\alpha = \frac{2a_0^6 e^{6\alpha}V_\ell}{\hbar^2}\left[\frac{\sqrt{3}\kappa|\beta|}{2}\right]^{-2} > 0.$$

The r^{-2} potential in quantum mechanics was discussed, for example, in [44–46]; cf. also [47] and the references therein. It became recently of interest in studying the polymer quantization which is motivated by loop quantum gravity [47].

Note that for the models with a big-freeze singularity we then have $\beta \ll -1$, whereas for the model with a big-démarrage singularity we have $\beta \gg 1$. We expect that this case is sufficiently generic to accommodate also the fea-

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[9]In fact, there is one such equation for positive and one for negative ϕ. Both equations are (due to the modulus dependence of the potential) identical. Matching is carried out through the conditions $\Psi_+(0) = \Psi_-(0)$ and $\Psi_+'(0) = -\Psi_-'(0)$, where $\Psi_\pm$ refer to the positive/negative ϕ solutions, respectively. These conditions imply that the constants in both solutions coincide. We will therefore just refer to the modulus-dependent equation (29) and its solution, keeping in mind that we have the same solution for positive and negative ϕ.

tures of other singular potentials. As is known from quantum mechanics [44,45], the most important issue for singular potentials is the fact that square integrability no longer suffices to select a unique class of states and that the spectrum therefore contains an ambiguity. This ambiguity points to new physics at short scales and must be fixed by either experiment or knowledge from a more fundamental theory. It is the fortunate property of the Coulomb potential that its ensuing states do *not* contain such an ambiguity (see, however, [48]). Thus, for the least singular potential, which is realized for $|\beta| \gg 1$, we have to solve the equation

$$\varphi_k'' + \left[\ell k^2 + \frac{\tilde{V}_\alpha}{|\phi|^2} \right] \varphi_k = 0. \tag{30}$$

Note that phantom and scalar matter have to obey the same quantum equation,[10] where the realm of positive energy for the ordinary scalar field $k^2 > 0$ corresponds to the realm of negative energy for the case of the phantom field $k^2 < 0$; cf. Eq. (29). The general solution to this equation is given by [49]

$$\varphi_k(\alpha, |\phi|) = \sqrt{|\phi|}[c_1 J_\nu(\sqrt{\ell}k|\phi|) + c_2 Y_\nu(\sqrt{\ell}k|\phi|)], \tag{31}$$

where $\nu := \sqrt{(1/4) - \tilde{V}_\alpha}$, so the index is a function of α. There are four cases to distinguish: k can be real or imaginary, depending on whether the energy entering k^2 is positive or negative. Furthermore, ν can be real or imaginary, depending on the parameters β, A, and the value of α. Note that φ_k satisfies

$$\ell(k^2 - n^2) \int_0^b d\phi \varphi_k(\phi) \varphi_n(\phi)$$
$$= \left[\varphi_k(b) \frac{d\varphi_n}{d\phi}(b) - \varphi_n(b) \frac{d\varphi_k}{d\phi}(b) \right], \tag{32}$$

where $b = \infty$ for the standard scalar field and $b = \phi_\star := \frac{\pi}{2}(2/\sqrt{3}\kappa|1 + \beta|)$ for the phantom scalar field. [This equation is analogous to Eq. (11) in [45].] We have fixed the range of definition for ϕ in the phantom case from 0 to $\phi_\star$ because all classical solutions are restricted to this range. That this also holds in the quantum theory is, of course, an assumption, similar to treating, say, a particle on the half-line only.

The lower bound in the integral (32) does not contribute as φ_k vanishes at the origin (see below). Thus the matter-dependent part of the wave function is not necessarily orthogonal. But it is if the right-hand side of (32) vanishes. This is the case if $b = \infty$ and ν is not an integer, as happens for the standard scalar field. The reason is the following: (i) The first Bessel function J_ν satisfies an orthogonality

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[10]Note that $V_1 = \frac{|A|^{1/(1+\beta)}}{2}$ and $V_{-1} = \frac{A^{1/(1+\beta)}}{2}$, so both are positive and coincide numerically.

relation, and (ii) the $J_\nu(\sqrt{\ell}k|\phi|)$ and $J_{-\nu}(\sqrt{\ell}k|\phi|)$ are linearly independent solutions of (30) (except when ν is an integer). Therefore, as the solution φ_k can then be expressed exclusively in terms of the first kind of Bessel functions, φ_k is orthogonal if either of the two coefficients in front of $J_\nu(\sqrt{\ell}k|\phi|)$ or $J_{-\nu}(\sqrt{\ell}k|\phi|)$ is zero. Otherwise, that is, if ν is an integer, additional conditions have to be imposed to get orthogonal eigenfunctions, as is the case for the phantom scalar field.

Different types of solutions for the three models discussed in our paper will differ by the boundary conditions that we may choose to impose (see next section). This choice is determined by the classical trajectory. For ordinary matter the classical trajectory has a minimum (see Fig. 2), whereas for phantom matter with $\beta + 1 < 0$ it reaches its maximum at the classical singularity (see Fig. 3). For the second phantom model with $\beta > 0$, the singularity lies again at a minimum of the classical trajectory. We will see how this difference in the classical model influences the quantum behavior through the boundary condition. Moreover, the phantom field is restricted to a finite range.

Independent of boundary conditions, the singularity occurs in all three models at $\phi = 0$ and $\alpha = 0$. For $\alpha = 0$, $\nu = \nu_0 := \sqrt{(1/4) - \tilde{V}_{\alpha=0}}$. There are three cases to distinguish: $\frac{1}{4} - \tilde{V}_{\alpha=0} > 0$, $\frac{1}{4} - \tilde{V}_{\alpha=0} < 0$, and the transitional case $\frac{1}{4} - \tilde{V}_{\alpha=0} = 0$. In the first and third cases ν_0 is real, whereas in the second case it is purely imaginary.

(i) $\frac{1}{4} - \tilde{V}_{\alpha=0} > 0$.—Then $0 < \nu < \frac{1}{2}$. In the quantum mechanical analogy, this corresponds to the case of a regular potential. We get from the behavior of the first Bessel function for a small argument

$$J_\nu(z) \approx \left(\frac{z}{2}\right)^\nu \frac{1}{\Gamma(\nu + 1)}, \qquad \nu \neq -1, -2, -3 \ldots \tag{33}$$

[cf. [49], Eq. (9.1.7)] that it vanishes at the origin. This holds for the real as well as imaginary argument. The behavior of the second Bessel function for a small argument is given by

$$Y_\nu(z) \approx -\frac{1}{\pi}\left(\frac{z}{2}\right)^{-\nu} \Gamma(\nu), \qquad \text{Re}(\nu) > 0 \tag{34}$$

[cf. [49], Eq. (9.1.9)]. Thus it diverges weaker than $|\phi|^{-1/2}$. As the Bessel functions in φ_k are multiplied by a factor $\sqrt{|\phi|}$, this divergence is, however, cancelled. We thus conclude that the matter-dependent part of the wave function vanishes at the singularity. In the quantum mechanical case of regular potentials, one of the two independent solutions of the Schrödinger equation is not normalizable and therefore discarded. This is, however, not necessarily the case for a vanishing angular momentum, since for the Coulomb potential, for example, both solutions

are normalizable. The selection occurs in that case because only one of the solutions leads to an essential self-adjoint Hamiltonian [50]. Such an argument can, however, not be invoked in the present case because the classical time parameter t is absent in quantum cosmology. There is thus no notion of unitarity here and thus no reason to advocate the self-adjointness of the Hamiltonian. We thus have nonuniqueness also in the "regular" case.

(ii) $\frac{1}{4} - \tilde{V}_{\alpha=0} < 0$.—This corresponds to the singular case in quantum mechanics. Here, ν_0 is imaginary; we write $\nu_0 = i\nu_0$. Since the above formula (33) holds for $\nu \neq -1, -2, -3 \ldots$, we can still use it and find

$$\lim_{|\phi| \to 0} \sqrt{|\phi|} J_{i\nu_0}(\sqrt{\ell}|\phi|k) = \lim_{|\phi| \to 0} \sqrt{|\phi|} \frac{1}{\Gamma(1 + i\nu_0)} \times e^{i\nu_0 \ln(\sqrt{\ell}k|\phi|/2)}. \quad (35)$$

For real as well as imaginary k (corresponding to positive and negative energy, respectively), this part of the matter-dependent wave function oscillates infinitely rapidly as it goes to zero as $|\phi| \to 0$. For the second part of the matter-dependent wave function, we introduce a small parameter $\epsilon > 0$, since (34) holds only for $\text{Re}(\nu) > 0$:

$$\lim_{|\phi| \to 0} \lim_{\epsilon \to 0} \sqrt{|\phi|} Y_{\epsilon+i\nu}(|\phi|\sqrt{\ell}k)$$

$$= -\frac{1}{\pi} \lim_{|\phi| \to 0} \lim_{\epsilon \to 0} \sqrt{|\phi|} \left(\frac{\sqrt{\ell}k|\phi|}{2}\right)^{-\epsilon} \quad (36)$$

$$\times \Gamma(\epsilon + i\nu_0) e^{i\nu_0 \ln(\sqrt{\ell}k|\phi|/2)}.$$

This function oscillates very rapidly but goes to zero as $|\phi| \to 0$ due to the factor $\sqrt{|\phi|}$. We therefore conclude that the wave function vanishes at the origin in this parameter range as well.

(iii) $\frac{1}{4} - \tilde{V}_{\alpha=0} = 0$.—In this case we have to consider the Bessel functions $J_0(z)$ and $Y_0(z)$ for small z. It is $J_0(0) = 1$ and so this part of φ_k vanishes when multiplied by $\sqrt{|\phi|}$ for $\phi \to 0$. But $Y_0(z) \approx \frac{2}{\pi} \ln(z)$ for small z [see [49], Eq. (9.1.8)] and thus diverges but $\sqrt{z} Y_0(z) \approx \frac{2}{\pi} \sqrt{z} \ln(z) \to 0$ as $z \to 0$. We thus find a vanishing wave function in this case as well.

The singularities in these three cases are thus avoided when the matter-dependent part of the wave function vanishes. To complete this claim, we have to ensure that the gravitational part of the wave function does not diverge at the respective singularities. Note that this result does not depend on any boundary conditions but is just a consequence of the Wheeler-DeWitt equation.

Note also that the general solution φ_k does not vanish at the singularity if $\nu = \frac{1}{2}$. This corresponds to $V_\ell = 0$, thus a vanishing potential. This case is excluded by the setup of our model. One could read this as: no potential implies no

singularity and thus no singularity avoidance but a finite wave function at the origin $\phi = 0$. Nevertheless, it is always possible to pick up a specific solution, that is, a particular φ_k which vanishes.

Concerning the gravitational part of the wave function, inserting the solution (31) for the matter-dependent part of the wave function into the Wheeler-DeWitt equation (24), we arrive at

$$\frac{\kappa^2}{6}(2\dot{C}_k\dot{\varphi}_k + C_k\ddot{\varphi}_k) + \left(\frac{\kappa^2}{6}\ddot{C}_k + k^2 C_k\right)\varphi_k = 0, \quad (37)$$

where a dot denotes derivative with respect to α. To obtain the gravitational part of the wave function, we assume that the terms $\dot{C}_k\dot{\varphi}_k$ and $C_k\ddot{\varphi}_k$ can be neglected; this is just the meaning of the Born-Oppenheimer approximation discussed above. Basically, we assume that C_k varies much more rapidly with α than φ_k and, moreover, neglect the backreaction of the matter part on the gravitational part. In summary, we are assuming that the change in the matter part does not influence the gravitational part; the matter part simply contributes its energy through k^2. This leads to the equation

$$\left(\frac{\kappa^2}{6}\ddot{C}_k + k^2 C_k\right)\varphi_k = 0. \quad (38)$$

It is solved by

$$C_k(\alpha) = b_1 e^{i(\sqrt{6}k/\kappa)\alpha} + b_2 e^{-i(\sqrt{6}k/\kappa)\alpha}. \quad (39)$$

As the equation determining the gravitational part of the wave function is independent of ℓ, we get the same solution, irrespective of whether we deal with a phantom or with a scalar field. Note that for $k^2 < 0$, k becomes imaginary and the dependence on α becomes exponential. In any case, $C_k(\alpha = 0) < \infty$, so the wave function remains finite at the respective singularities and we can safely speak of singularity avoidance.

V. BOUNDARY CONDITIONS AND SINGULARITY AVOIDANCE

Nobody knows what the correct boundary condition for the quantum universe is. There have been several proposals, most of them using the boundary condition with the ambition to lead to singularity avoidance [43,51–53]. DeWitt, in particular, speculates that the fact that a boundary condition is generally needed to make the quantum theory "singularity-free: is an argument in favor of the theory: The theory itself does not leave any freedom of choice but provides the boundary condition itself [43]. As for the present state of understanding quantum gravity, however, singularity avoidance is demanded from the outside as a selection criterion.

Irrespective of this discussion, it is in general necessary to impose a completely *different* condition if one instead wants to construct wave packets that follow classical tra-

jectories with a turning point in configuration space [42]. Namely, one has to require that the wave packet decays in the classically forbidden region. This allows the interference of wave packets following the two branches of the classical solution behind the classical turning point. Of course, this is just the standard quantum mechanical treatment of classically forbidden regions. In general, out of solutions to the Wheeler-DeWitt equation which grow in the classically forbidden region, no wave packet can be constructed that follows the classical path. This is what happens generically for the no-boundary state [54]. In order to make connection with the underlying classical theory, we shall therefore use herein as a condition that the wave function decrease in the classically forbidden region.

One cannot assume that the condition of the wave function to decrease into the classically forbidden region always fixes it uniquely. Nonetheless, it is a necessary condition that has to be imposed in order to get a theory with the correct semiclassical limit. It can be used in selecting physically sensible solutions out of the general set of solutions to the Wheeler-DeWitt equation. We now want to explore the situation for our models presented above.

A. Defrosting the big freeze

1. Standard scalar field

In the classical scalar-field model, the region $a < a_{\min} = 1$ is a forbidden region.[11] We impose the boundary condition that the wave function decay there. In terms of the variable α, the boundary condition to be imposed is therefore $\Psi \to 0$ as $\alpha \to -\infty$. But as $\alpha \to -\infty$, $\nu \to \frac{1}{2}$. The matter-dependent part of the wave function is then given by

$$\lim_{\alpha \to -\infty} \varphi_k(\alpha, |\phi|) = \sqrt{\frac{2}{\pi}}[c_1 \sin(k|\phi|) - c_2 \cos(k|\phi|)];$$

$$(40)$$

see [49], Eqs. (10.1.11) and (10.1.12). This vanishes for small $|\phi|$ if $c_2 = 0$ for both real and imaginary k. Thus imposing $c_2 = 0$, we are left with the solution[12]

$$\varphi_k(\alpha, |\phi|) = c_1 \sqrt{|\phi|} J_\nu(k|\phi|). \qquad (41)$$

Because of the vanishing of φ_k at the origin and its boundedness at infinity, the φ_k are orthogonal, that is, $\int d\phi \varphi_k \varphi_n \propto \delta(k - n)$ [55]. This is due to the fact that ϕ can become arbitrarily large. If the integration range of ϕ was finite, we would need additional conditions to ensure

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[11]Recall that we use $\tilde{a} = \frac{a}{a_{\max}}$ and drop the tilde.
[12]In the quantum mechanics of a repulsive r^{-2} potential, $r^{1/2} J_\nu(kr)$ is the unique solution which vanishes at $r = 0$; cf. Eq. (3.3) in [44].

orthogonality; cf. [49], Eq. (11.4.5). Despite the orthogonality, k is not restricted to be of integer value.

Inserting the solution (41) for the matter-dependent part of the wave function into the Wheeler-DeWitt equation (24), we arrive at (37). To obtain the gravitational part of the wave function, we proceed as before and find (39) for the gravitational part of the wave function.

For positive energy $k^2 > 0$, the gravitational part of the wave function is thus oscillating. No further complications arise, and the full solution is given by

$$\Psi_k(\alpha, \phi) = c_1 \sqrt{|\phi|} J_\nu(k|\phi|) [b_1 e^{i(\sqrt{6}k/\kappa)\alpha}$$
$$+ b_2 e^{-i(\sqrt{6}k/\kappa)\alpha}]. \qquad (42)$$

For negative energy, however, the gravitational part becomes exponential. To ensure that the boundary condition $\Psi \to 0$ as $\alpha \to -\infty$ is satisfied for the entire wave function, we have to set $b_1 = 0$. Thus, for imaginary k the gravitational part of the wave function decays exponentially for $\alpha \to -\infty$, whereas the matter part remains finite; see Eq. (41). The gravitational part alone ensures in this way that the wave function vanishes as $\alpha \to -\infty$. No additional condition arises for φ_k. The full solution for imaginary $k \to ik$ is thus

$$\Psi_k(\alpha, \phi) = b_2 e^{(\sqrt{6}k/\kappa)\alpha} [c_1 J_\nu(ik|\phi|) + c_2 Y_\nu(ik|\phi|)],$$
$$(43)$$

and φ_k and φ_n are not orthogonal in this case.

Notice that the functions $\Psi_k(\alpha, \phi)$ given in (42) and (43) fulfil as well the DeWitt criterion as they vanish for $\alpha = 0$ and $\phi = 0$.

2. Phantom scalar field

The classical model with the phantom-driven generalized Chaplygin gas has a classically forbidden region given by $a > a_{\max} = 1$. We therefore impose the boundary condition $\Psi \to 0$ as $\alpha \to \infty$. In this limit, ν becomes purely imaginary and large. We shall set here $\nu := i\nu$ and $\nu \to \infty$ (ν now being real). We are thus looking for a combination of Bessel functions which vanish for a large imaginary index.

The wave function for positive energies, that is, $k^2 > 0$, can be written as

$$\varphi_k(\alpha, |\phi|) = \sqrt{|\phi|}[c_1 J_{i\nu}(ik|\phi|) + c_2 Y_{i\nu}(ik|\phi|)]. \quad (44)$$

As in this case the argument of the Bessel functions is purely imaginary, it is rather convenient to rewrite the wave function in terms of the linearly independent modified Bessel functions [49]:

$$\varphi_k(\alpha, |\phi|) = \sqrt{|\phi|}[\tilde{c}_1 I_{i\nu}(k|\phi|) + \tilde{c}_2 K_{i\nu}(k|\phi|)], \quad (45)$$

where $\tilde{c}_1$ and $\tilde{c}_2$ are arbitrary constants. It can be shown that the modified Bessel function $K_{i\nu}(k|\phi|)$ goes asymp-

totically to zero as $\nu \to \infty$ by using

$$K_{i\nu} = \sqrt{2}(\nu^2 - x^2)^{-1/4} \exp\left(-\frac{\nu}{2}\pi\right)$$
$$\times [\text{const} + \mathcal{O}((\nu^2 - x^2)^{-1/2})], \qquad \nu > x > 0; \quad (46)$$

cf. [56], Eq. (7.13.2(19)). Indeed, the modulus of the function $K_{i\nu}(k|\phi|)$ is oscillatory and its local extremum goes to zero as $\nu \to \infty$. Therefore, the implementation of the boundary condition gives

$$\varphi_k(\phi) = \tilde{c}_2 \sqrt{|\phi|} K_{i\nu}(k|\phi|). \quad (47)$$

On the other hand, the wave function for negative energies, that is, $k^2 < 0$, can be written as

$$\varphi_k(\alpha, |\phi|) = \sqrt{|\phi|}[c_1 J_{i\nu}(\tilde{k}|\phi|) + c_2 Y_{i\nu}(\tilde{k}|\phi|)], \quad (48)$$

where $\tilde{k} = ik$ and is positive. Here again it is more convenient to rewrite the general matter wave function in terms of Hankel functions in order to impose the boundary condition. We then rewrite the previous wave function as

$$\varphi_k(\alpha, |\phi|) = \sqrt{|\phi|}[d_1 H_{i\nu}^{(1)}(\tilde{k}|\phi|) + d_2 H_{i\nu}^{(2)}(\tilde{k}|\phi|)], \quad (49)$$

where d_1 and d_2 are arbitrary constants to be fixed by the boundary condition. It can be checked that $H_{i\nu}^{(1)}(\tilde{k}|\phi|)$ diverges for large ν because

$$H_{i\nu}^{(1)}(x) = \frac{\sqrt{2}}{\pi}(\nu^2 + x^2)^{-1/4} \exp\left[i\sqrt{\nu^2 + x^2} - i\nu \operatorname{arcsinh}\left(\frac{\nu}{x}\right)\right]$$
$$\times \exp\left[\frac{\pi}{2}\nu - i\frac{\pi}{4}\right][\text{const} + \mathcal{O}((\nu^2 + x^2)^{-1/2})],$$
$$\nu, x > 0; \quad (50)$$

cf. [56], Eq. (7.13.2(22)). On the other hand, it can be shown that $H_{i\nu}^{(2)}(\tilde{k}|\phi|)$ vanishes at large values of ν. This can be shown by combining the following properties of the Hankel functions: $H_{i\nu}^{(2)}(x) = \exp(-\pi\nu)H_{-i\nu}^{(2)}(x)$ and $H_{-i\nu}^{(2)}(x) = (H_{i\nu}^{(1)}(x))^\star$, where $\star$ denotes complex conjugation, and the asymptotic expansion of $H_{i\nu}^{(1)}(x)$ for large order as shown above. Therefore, the wave function that fulfils the boundary condition for negative energies reads

$$\varphi_k(\alpha, |\phi|) = d_2 \sqrt{|\phi|} H_{i\nu}^{(2)}(\tilde{k}|\phi|). \quad (51)$$

Before proceeding further, it is worthwhile to point out the following. The ordinary scalar field is defined on the entire real line. The phantom field, on the other hand, is restricted to the interval $|\phi| \in [0; \phi_\star]$. Orthogonality therefore does not hold straightaway but follows only if Eq. (32) is satisfied in the boundaries in which ϕ is defined. To obtain orthogonality, additional conditions would be necessary. As we cannot require that φ_k vanishes at $\phi_\star$, as this would be in conflict with the requirement that the wave function follows the classical trajectory, we have to

demand that its derivative with respect to ϕ vanish there. This would require an analytic expression of the zeros of the first derivative of the modified Bessel function $K_{i\nu}$ and the second Hankel function. To our knowledge, such an expression does not exist. Also, there is no *physical* motivation for this additional condition.

The C_k have to satisfy $\frac{\kappa^2}{6}\ddot{C}_k + k^2 C_k = 0$. The solution is given by Eq. (39): (i) For positive energy, the imposition of the boundary condition leaves b_1 and b_2 as arbitrary constants, and therefore we need to impose the boundary condition on the matter-dependent part in this case; see Eq. (47). (ii) For negative energy, the imposition of the boundary condition picks up the exponentially decreasing function. The decay of the wave function for large α is thus already guaranteed through the purely gravitational part of the wave function. In principle, there is no need to impose the boundary condition on the matter-dependent part in this case, as long as the general solution for the matter part is finite. However, it is not the case, so we have as well to impose the boundary condition on the matter part. This implies that only the second kind of Hankel function $H_{i\nu}^{(2)}$ is present on the matter part [see Eq. (51)].

In summary, the physical solutions are

$$\Psi_k(\alpha, \phi) = (b_1 e^{i(\sqrt{6}k/\kappa)\alpha} + b_2 e^{-i(\sqrt{6}k/\kappa)\alpha})\sqrt{|\phi|}K_{i\nu}(k|\phi|),$$
$$k^2 > 0,$$

$$\Psi_k(\alpha, \phi) = d_2 \exp\left(-\frac{\sqrt{6}}{\kappa}\tilde{k}\alpha\right)\sqrt{|\phi|}H_{i\nu}^{(2)}(\tilde{k}|\phi|),$$
$$k^2 < 0. \quad (52)$$

These restrictions have to be taken into account when constructing wave packets (which will not be attempted here). Before concluding this subsection, we remark that the functions $\Psi_k(\alpha, \phi)$ given in (52) fulfil the DeWitt criterion as well, since they approach zero for $\alpha = 0$ and $\phi = 0$.

B. Smoothing the big-démarrage singularity

As a third model with the same quantum structure, we consider the big-démarrage singularity. The equations for this singularity as it occurs for $\beta \gg 1$ are just the same as for the big freeze generated by a phantom GCG presented above. The solution is also given by Eq. (31). The difference lies in the classically forbidden region and thus in the boundary condition to be employed. Whereas in the previously studied phantom model we found a future singularity at $a = a_{\max}$, this model has a past sudden singularity at $a = a_{\min} = 1$. We therefore require the wave function to satisfy $\Psi \to 0$ as $\alpha \to -\infty$. But as $\alpha \to -\infty$, $\nu \to \frac{1}{2}$.

We split our analysis for positive and negative energies. For $k^2 > 0$, the boundary condition on the matter part of the wave function is $c_1 = 0$; that is, we are left with the first Bessel function, while the gravitational part will be oscillatory. On the other hand, for $k^2 < 0$, the boundary condi-

tion on the gravitational part of wave function implies $b_1 = 0$, while no other boundary condition has to be imposed on the matter sector of the wave function. In summary, we obtain

$$\Psi_k(\alpha, \phi) = (b_1 e^{i(\sqrt{6}k/\kappa)\alpha} + b_2 e^{-i(\sqrt{6}k/\kappa)\alpha})\sqrt{|\phi|}J_\nu(ik|\phi|),$$
$$k^2 > 0,$$

$$\Psi_k(\alpha, \phi) = \exp\left(\frac{\sqrt{6}}{\kappa}k\alpha\right)\sqrt{|\phi|}[c_1 J_\nu(\tilde{k}|\phi|) + c_2 Y_\nu(\tilde{k}|\phi|)],$$
$$k^2 < 0, \qquad (53)$$

where $\tilde{k} = ik$.

The solution is thus similar to the one found for the standard scalar GCG presented in the previous subsection. But note that ϕ is restricted to a finite interval here.

Furthermore, as a consequence of the fact that the phantom scalar field has compact range, the matter-dependent part of the wave function φ_k is not orthogonal for different k. To obtain this, one has to require the condition (32).

Here as well we notice that the functions $\Psi_k(\alpha, \phi)$ given in (53) fulfil the DeWitt criterion as they vanish at $\alpha = 0$ and $\phi = 0$.

C. Other boundary conditions

The Schrödinger equation with inverse-square potential has been studied by various authors [44,45]. They obtain as a solution the Hankel function of the first kind, $H_\nu^{(1)}$ for $k^2 < 0$ and $\tilde{V}_\alpha > \frac{1}{4}$; cf. Eq. (3.6) in [44]. Therefore, their solution is different from the ones we have obtained in the previous subsections. This is due to the boundary condition that is imposed in quantum mechanics: $\Psi \to 0$ as $r \to \infty$, r being the radial coordinate in the Schrödinger equation. In the quantum-cosmological model, this would correspond to the condition $\Psi \to 0$ as $|\phi| \to \infty$. Whereas the vanishing of the wave function at infinity is a sensible requirement in quantum mechanics, it is not well-motivated in quantum cosmology. To demand a square-integrable wave function makes sense only in a Hilbert space with a probability interpretation and a (time) conserved probability. It is not obvious that we have such a structure in quantum cosmology: The Wheeler-DeWitt equation is timeless.

Applying nevertheless this boundary condition to the quantum-cosmological model with GCG mimicked by a standard scalar field,[13] we find $\varphi_k(\alpha, \phi) = c_1\sqrt{|\phi|}H_\nu^{(1)}(i\tilde{k}|\phi|)$, with $\tilde{k}^2 = -k^2$ and ν purely imaginary as $\tilde{V}_\alpha > \frac{1}{4}$. This wave function corresponds to the choice $c_2 = ic_1$. Requiring in addition orthogonality as in [44], we would arrive at an energy spectrum given by

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[13]Notice that the boundary condition imposed in [44,45] cannot be applied in our model with a phantom scalar field. The reason is that the scalar field is bounded in this case, so we cannot take the limit $|\phi| \to \infty$ in $\varphi_k(\alpha, \phi)$.

$$E_n(\alpha) = -\frac{\hbar^2 \kappa_0^2}{2} \exp\left(\frac{2\pi n}{\sqrt{\tilde{V}_\alpha - \frac{1}{4}}}\right), \qquad n \in \mathbb{Z}, \qquad (54)$$

where κ_0 is an *arbitrary* real constant. This can be done only for $k^2 < 0$. This is a similar nonuniqueness as in the quantum mechanical case [44].

Now we can impose two different types of boundary condition on the total wave function Ψ:
(1) C_k vanishes at the singularity; i.e. at $\alpha \approx 0$, and $\varphi_k(\alpha, \phi)$ is bounded at $\alpha \approx 0$ and $\phi \approx 0$, or
(2) C_k vanishes well inside the forbidden region; i.e. $\alpha \to -\infty$, and $\varphi_k(\alpha, \phi)$ is bounded for $\alpha \to -\infty$ and $\phi \approx 0$. We next impose both conditions separately.

The equation for the gravitational part of the general solution for the wave function obtained through a Born-Oppenheimer approximation [see Eq. (38)] can then be solved in the vicinity of the singularity, i.e. for $\alpha \approx 0$. It satisfies

$$\ddot{C}_k - \gamma(1 - \delta\alpha)C_k = 0, \qquad (55)$$

where the constants γ, δ, and c read, respectively,

$$\gamma = \frac{6\kappa_0^2}{\kappa^2} \exp\left[\frac{4\pi n}{\sqrt{4c - 1}}\right], \qquad \delta = \frac{48\pi nc}{(4c - 1)^{3/2}},$$
$$c = \frac{2}{\hbar^2} a_0^6 V_\ell\left[\frac{\sqrt{3}}{2}\kappa|1 + \beta|\right]^{-2}. \qquad (56)$$

Therefore, the gravitational part of the wave function for $\alpha \approx 0$ reads [49]

$$C_k(\alpha) = b_1\text{Ai}\left[\left(\frac{\gamma}{\delta^2}\right)^{1/3} - (\delta\gamma)^{1/3}\alpha\right]$$
$$+ b_2\text{Bi}\left[\left(\frac{\gamma}{\delta^2}\right)^{1/3} - (\delta\gamma)^{1/3}\alpha\right], \qquad (57)$$

where $\text{Ai}(z)$ and $\text{Bi}(z)$ denote Airy functions. Imposing that the wave function C_k vanishes at the singularity ($\alpha = 0$) implies

$$b_2 = -b_1 \frac{\text{Ai}[(\frac{\gamma}{\delta^2})^{1/3}]}{\text{Bi}[(\frac{\gamma}{\delta^2})^{1/3}]}. \qquad (58)$$

It can be proven as well that $\varphi_k(\alpha, \phi) = c_1\sqrt{|\phi|}H_\nu^{(1)}(i\tilde{k}|\phi|)$ vanishes for $\alpha \approx 0$ and $\phi \approx 0$. Therefore, we can conclude that the DeWitt criterion is compatible (in this case) with the boundary condition used in [44,45].

The boundary condition $\Psi \to 0$ as $\alpha \to -\infty$ cannot be imposed on the previous wave function (57). This is so because the wave function (57) is valid only around $\alpha \approx 0$. In order to impose the boundary condition $\Psi \to 0$ as $\alpha \to -\infty$, we have to consider the wave function for $\alpha \to -\infty$. In this limit, the energy spectrum (54) reduces to[14]

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[14]In taking this limit, notice that $E_n(\alpha)$ can become complex. However, $E_n(\alpha)$ given in (59) is always positive.

$$E_n(\alpha) = -\frac{\hbar^2 \kappa_0^2}{2}. \qquad (59)$$

Consequently,

$$C_k(\alpha) = b_1 \exp\left(\frac{\sqrt{6}\kappa_0}{\kappa}\alpha\right) + b_2 \exp\left(-\frac{\sqrt{6}\kappa_0}{\kappa}\alpha\right). \qquad (60)$$

Now the condition $C_k \to 0$ as $\alpha \to -\infty$ implies $b_2 = 0$. On the other hand, $\varphi_k(\alpha, \phi) = c_1\sqrt{|\phi|}H_\nu^{(1)}(i\tilde{k}|\phi|)$ is bounded for $\alpha \to -\infty$ and $\phi \approx 0$. Therefore, we can conclude that the condition $\Psi \to 0$ as $\alpha \to -\infty$ is fulfilled and compatible with the boundary condition used in [44,45].

In summary, as the wave function remains finite, the singularity would be avoided with the boundary conditions 1 and 2 as well. But we emphasize again that the condition $\Psi \to 0$ as $|\phi| \to \infty$ is perhaps not obligatory in the quantum-cosmological case. It is presented here to compare our results to results presented elsewhere in the literature.

VI. CONCLUSIONS AND OUTLOOK

What are the main results of our paper? We have shown how the classical singularities of particular cosmological models describing dark-energy features can be avoided in quantum cosmology. The framework is quantum geometrodynamics, and restriction has been made to a class of models (containing a generalized Chaplygin gas) which could be of relevance for the description of dark energy. The wave function Ψ is defined on a two-dimensional configuration space consisting of the scale factor a and the scalar field ϕ representing the gas. After employing a Born-Oppenheimer type of approximation, we arrive at an effective stationary Schrödinger equation with singular (in the sense of quantum mechanics) potentials. The occurrence of such potentials in quantum mechanics signals an essential nonuniqueness of the solutions. The same happens here. Requiring that the wave function go to zero in the classically forbidden region still leaves a whole class of solutions which encode singularity avoidance in the sense of a vanishing wave function (DeWitt criterion). This is different from our earlier papers [18,24] in which we dealt with regular potentials and where appropriate normalizability assumptions singled out singular-free solutions (cf. also [19]). The case of the big-brake singularity in [24] contains a potential that behaves like the Coulomb potential in the vicinity of the classical singularity; as in quantum mechanics, no ambiguity remains after normalizability is being assumed.

Our analysis has been performed in detail only for the case of the r^{-2} potential. A similar discussion can be made for the r^{-4} potential leading to Mathieu functions; since the results are analogous to those of the r^{-2} potential, we do not present them here. We expect that a similar,

although much more complicated, analysis can be performed for other singular potentials as well. It would be desirable to have a general classification of singularities with respect to singularity avoiding states at hand.

We want to emphasize again one important conceptual aspect of this (and earlier) work. The singularities in these models do generally occur for a big universe, that is, for a value of the scale factor much bigger than the Planck scale. Singularity avoidance by quantum gravity then necessarily entails quantum effects for a big universe. Such quantum effects have been discussed earlier in the case of a classically recollapsing quantum universe [57]; the quantum effects occur there near the (nonsingular) region of the classical turning point as a consequence of the boundary conditions. We thus see that quantum cosmology may be of direct relevance for the future of our Universe. As discussed at length in [57], the occurrence of such quantum effects possesses essential importance for understanding the arrow of time. It would be of great interest to study the question of entropy increase in the present models.

There are many further open questions. In quantum mechanics, the remaining ambiguity of the solutions and the ensuing spectra point to new physics at short distances. The ambiguity must therefore be fixed either by reference to experimental results or by knowledge of the deeper theory. How is the situation in quantum cosmology? Experiments do not yet seem available, but can the ambiguity be fixed by theoretical means? One possible project would be to investigate whether prominent boundary conditions such as the no-boundary [51] or tunneling [52] conditions are able to fix it. Perhaps the ambiguity can be avoided only by going to a more fundamental theory such as string theory. On the other hand, it may as well be imaginable that cosmological models leading to such singular matter potentials have to be excluded—an interesting selection criterion for equations of state.

An essential ingredient in our whole analysis is the demand that the wave function go to zero in classically forbidden regions. How this relates in general to the hyperbolic structure of the Wheeler-DeWitt equation is not fully understood. Here we have avoided this problem by going to the Born-Oppenheimer approximation. In general, one would expect that certain quantization conditions on the physical parameters (masses, coupling constants, a cosmological constant) may appear [41,58–60]. It would also be very interesting to establish a connection with a group-theoretical generalization of quantum geometrodynamics where it was shown that not only time but even the ordinary three-dimensional space is absent at the most fundamental level, leading to singularity avoidance in a natural way [61]. We hope that we can address some of these open issues in future publications.

Finally, let us point out that a future sudden singularity has been recently investigated in [62]. The analysis was carried out in the loop quantum cosmology

(LQC) framework.[15] In this model, matter is modeled by a scalar field which rolls down (standard scalar field) or up (phantom scalar field) through an unbounded exponential potential. In the framework of LQC, this scalar field behaves such that its effective energy density is finite; that is, there is a balance between its kinetic energy and its potential, while the effective pressure blows up in a finite future cosmic time. It was then concluded in [62] that such a singularity cannot be avoided by means of the effective Friedmann equation in LQC. As it is mentioned in [62], the sudden singularity that appears for the phantom scalar field in the context of the modified Friedmann equation in LQC corresponds to a big-rip singularity in the standard relativistic case. For such a big-rip singularity, it was shown in [18] that it can be avoided in the sense that wave packets necessarily disperse when they approach the region of the classical big-rip singularity. It would be interesting to see if this sort of big-rip singularity can be avoided as well by employing the DeWitt criterion that the wave function be zero at the classical singularity.

ACKNOWLEDGMENTS

APPENDIX: JUSTIFICATION OF THE GRAVITATIONAL WAVE FUNCTION APPROXIMATION

In our models, we constructed the potential $V(\phi)$ such that it corresponds to the polytropic equation of state for a GCG. The potential therefore depends on κ, and this dependence carries over to the matter-dependent part of the wave function. The Born-Oppenheimer approximation can be understood as an expansion scheme with respect to κ.

The derivatives of φ_k with respect to α are of nonzero order in κ. This comes from $\dot{\varphi}_k = \frac{d\varphi_k}{d\nu^2}\frac{d\nu^2}{d\alpha}$. In the vicinity of the singularity, $\alpha \approx 0$ and $\frac{d\nu^2}{d\alpha} = -\frac{16}{\hbar^2}\frac{a_0^6}{\kappa^2}\frac{V_\ell}{|1+\beta|^2}$. Recall that $V_\ell = \frac{|A|^{1/(1+\beta)}}{2}$ and $a_0 = |\frac{B}{A}|^{1/3(1+\beta)}$. Recall also that we use ν_0 to denote the value of ν at $\alpha = 0$. Therefore

$$\frac{d\nu^2}{d\alpha} = -\frac{8}{\hbar^2\kappa^2}\left|\frac{B^2}{A}\right|^{1/(1+\beta)}\frac{1}{|1+\beta|^2}. \quad (A1)$$

From Eq. (39) we see that $C_k \sim \mathcal{O}(\kappa^0)$, $\dot{C}_k \sim \mathcal{O}(\kappa^{-1})$, and $\ddot{C}_k \sim \mathcal{O}(\kappa^{-2})$.

To obtain a consistent approximation scheme, such that in

$$\ddot{C}_k\varphi_k \sim \mathcal{O}(\kappa^{-2}), \quad \dot{C}_k\dot{\varphi}_k \sim \mathcal{O}(\kappa^{-1}), \quad C_k\ddot{\varphi}_k \sim \mathcal{O}(\kappa^1) \quad (A2)$$

only the first term is kept and the others neglected, we have to assume that $|\frac{B^2}{A}|^{1/(1+\beta)} \sim \kappa^2$, i.e. $\frac{d\nu^2}{d\alpha} \sim \mathcal{O}(\kappa^0)$.

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