Wheeler-DeWitt Universe Wave Function in the presence of stiff matter

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We study the Wheeler-DeWitt (WDW) equation close to the Big-Bang. We argue that an interaction dominated fluid (speed of sound equal to the speed of light), if present, would dominate during such an early phase. Such a fluid with $p = \rho \propto 1/a^6$ generates a term in the potential of the wave function of the WDW equation proportional to $-1/a^7$. This very peculiar quantum potential, which embodies a spontaneous breaking of dilatation invariance, has some very remarkable consequences for the wave function of the Universe: $\Psi(a)$ vanishes at the Big-Bang: $\Psi(0) = 0$; the wave function $\Psi(a)$ is always real; a superselection rule assures that the system is confined to $a \geq 0$ without the need of imposing any additional artificial barrier for unphysical negative $a$. These results do not depend on the operator-ordering problem of the WDW equation.

PACS numbers: 98.80.Bp,98.80.Qc,04.60.Ds
Keywords: Wheeler-DeWitt equation, quantum cosmology, wave function of the Universe

\textbf{Motivation:} At the very beginning of the Universe evolution, just after the big-bang, the energy density was extremely high. In a classical treatment, one has the so-called big-bang singularity: the energy density diverges when the scale factor $a$ defining the Friedmann-Robertson-Walker (FRW) metric vanishes. It is however well known that ‘classical’ general relativity (GR) is not sufficient, since at such an early stage the influence of Quantum Mechanics (QM) is expected to be large.

One of the first treatments of quantum gravity was put forward by Wheeler and DeWitt\textsuperscript{(1)}: it is a canonical approach, in which the Hamiltonian of general relativity is quantized, hence the wave function is a function of the (spacial) metric. A Schrödinger-like equation, called Wheeler-DeWitt (WDW) equation, emerges. Although we still do not know if this is the correct and/or the most efficient way to quantize gravity\textsuperscript{(2–4)}, it represents a useful approach to describe various problems in which both GR and QM merge. This is especially the case of quantum cosmology.

The WDW equation simplifies tremendously when a uniform and homogenous FRW Universe is considered: the wave function is solely function of the scale parameter $a$ [hence, $\Psi = \Psi(a)$], see e.g.\textsuperscript{(5,6)}. However, it is not clear what fixes the boundary conditions (if any) associated with the WDW equation and a long debate has emerged in this context: while Hartle and Hawking find, within the so-called no-boundary proposal, a real wave function\textsuperscript{(7)} (see also\textsuperscript{(8–10)}) containing both ingoing and outgoing waves, Vilenkin\textsuperscript{(11)} put forward a complex wave function corresponding solely to an outgoing wave. Usually, in such studies of the early time of the Universe, only the curvature and the constant cosmological terms are retained. For a recent description of the other possible components, such as matter and radiation, see Refs.\textsuperscript{(12,13)}. Indeed, the interest on the wave function of the Universe is very strong, as the recent lively and vibrating dispute on the effect of quantum gravitational perturbations in the early universe shows\textsuperscript{(14–16)}.

Besides the problem of the explicit form of the wave function mentioned above, there are other issue connected to the WDW equation: (i) What should be the wave function at the big-bang, $\Psi(0)$? It is non-vanishing for both the Hartle-Hawing and Vilenkin solutions mentioned above. (ii) How to implement the classical constraint $a \geq 0$? Usually, the transformation $a = e^{i\Omega}$ is performed\textsuperscript{(5)}, but this is merely a mathematical trick. (iii) Should the wave function be real or complex? (iv) Is there any influence of the so-called operator ordering problem?

In this work, we shall consider the effect of a stiff-matter interaction dominated gas, for which the pressure equalize the energy density, $p = \rho$ (the speed of sound is c, hence maximal).

Namely, whatever d.o.f. are present in the very early universe, their strong interactions could generate such a gas. Quite remarkably, recent studies on the most dense form of strongly interacting matter, taking place in the core of neutron stars, show that the speed of sound should be larger than $1/\sqrt{3}$ (the value for a non-interacting ultrarelativistic gas of massless particles) in order to explain the existence of massive neutron stars\textsuperscript{(18)}. The study of this causal limit is common in neutron stars, since it is the stiffest possible Equation of State (EoS) and it is useful to set the limit to the highest possible mass\textsuperscript{(19–21)}. Theoretically, it is well understood how such a gas emerges due to

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of the Universe. Of course, the use of a constant \( w \) fulfills the EoS where strong interactions [22]. Indeed, a component of the form \( w \) dominated Universe is found by setting \( 30\% \) of contribution to the present state of the expansion, the rest being the present cosmic inflation. A radiation component \( \phi \) and one should consider that a massless scalar field \( \phi(t, x) \) should actually generate a gas of the type \( p = \rho/3 \) when fluctuations are included.

In the realm of quantum cosmology, a fluid with \( p = \rho \) corresponds to a term of the type \(-1/a^2\) in the effective potential of the WDW equation. Such a potential, if present, necessarily dominates at small \( a \) (other possibilities are excluded since would violate causality). This is indeed a very peculiar quantum potential that breaks all our naive expectations for a quantum system, see Ref. [27] and also refs. [28, 29]. At a first sight, it seems that no bound state should exist, since, if one exists, a continuum of bound states, one for each negative energy, would also exist. At a closer inspection, the system is much more interesting and its detailed treatment imposes to render the Hamiltonian self-adjoint [27, 30]: if the attraction is below a certain critical value, there is a single bound state, but, above, there is an infinity of bound states (one of which with lower energy). In turn, this system provides a beautiful example of an anomaly: a characteristic length in the system emerges, which is in a sense similar to the development of the Yang-Mills energy scale in QCD.

Quite remarkably, the unexpected features of the potential \(-1/a^2\) in the WDW equation may help to relieve in an elegant way the problems of the WDW approach listed above: (i) The wave function vanishes at the big-bang: \( \Psi(a = 0) = 0 \). This condition reminds the old idea of DeWitt according to which a vanishing wave function could represent a solution of the problem of the singularity [1, 3]. (ii) It generates a superselection rule according to which only positive (or negative) values of \( a \) are allowed. Hence, once \( a > 0 \) is chosen, the wave function is automatically nonzero only on the r.h.s. and there is no need of any further artificial restriction. (iii) The wave function is real in agreement with the result of Hartle and Hawking [7]. (iv) The results are qualitatively independent on (a very large class of) choice(s) of the operator ordering.

**WDW equation in cosmology:** We briefly review how the WDW equation emerges in cosmology. First, we consider the scale factor \( a = a(t) \) as a field with dimension length subject to the classical Lagrangian

\[
L_{\text{FRW}} = -Ca^3 \left[ \left( \frac{\dot{a}}{a} \right)^2 - \frac{k c^2}{a^2} + \frac{\Lambda c^2}{3} + \frac{8\pi G}{3c^2} \rho \right] \quad \text{with} \quad C = \frac{3\pi c^2}{4G},
\]

where \( k \) and \( \Lambda \) parametrize the curvature and the cosmological constant contributions to the Universe’s evolution.

The energy density \( \rho \) describes the contribution of matter and energy. Here, we shall consider that each component fulfills the EoS \( p = w \rho \), which has a constant speed of sound \( v_{\text{sound}} = c \sqrt{dp/d\rho} = c \sqrt{w} \leq c \). The adiabatic expansion \( dE + pdV = 0 \) translates into \( d(\rho a^3) + pd(a^3) = 0 \), then:

\[
a \frac{dp}{da} = -3(\rho + p) = -3(1 + w)\rho \implies \rho(a) = \frac{A_w}{a^{3(w+1)}}. \tag{2}
\]

As renowned [31], for \( w = 0 \) a Universe dominated by dust is obtained (\( \rho_{\text{dust}} \propto a^{-3} \), dark plus visible matter, about 30\% of contribution to the present state of the expansion, the rest being the present cosmic inflation). A radiation dominated Universe is found by setting \( w = 1/3 \) (\( \rho_{\text{radiation}} \propto a^{-4} \)); this was relevant in the radiation dominated era of the Universe. Of course, the use of a constant \( w \) is an approximation, since a relativistic plasma with \( w \approx 1/3 \) turns into a nonrelativistic gas \( w \approx 0 \) when the Universe cools down. Moreover, at a given time, different disjunct components of the fluid can follow their own EoS, leading to

\[
\rho = \rho_{\text{dust}} + \rho_{\text{radiation}} + \ldots \tag{3}
\]

Here, we argue that at the very beginning of the Universe, an interaction dominated gas whose EoS is given by \( w = 1 \) could have been present (whatever d.o.f. were relevant, see e.g. Ref. [32] and refs. therein). For this fluid:

\[
p = \rho \rightarrow v_{\text{sound}} = 1 \quad \text{and} \quad \rho_{\text{int-dom}} = \frac{A_{\text{int-dom}}}{a^6}.
\]

Clearly, this component can be relevant only at a very stage of the expansion, since (i) it decreases very fast for increasing \( a \) and (ii) the strong interaction generating it weakens down and transforms this fluid into a more conventional component [hence, \( w \) decreases from 1 to 1/3 (or even smaller)].

The first Friedmann equation is obtained by imposing that the Hamiltonian vanishes:

\[
H_{\text{FRW}} = \rho\dot{a} - L_{\text{FRW}} = 0 \quad \text{with} \quad \dot{a} = \frac{\partial L_{\text{FRW}}}{\partial \dot{a}} - 2Ca\dot{a}. \tag{5}
\]
This constraint follows from the invariance under coordinate transformations of GR. In terms of $a$ and $\dot{a}$, Eq. (5) gives the first Friedmann equation

$$\left(\frac{\dot{a}}{a}\right)^2 + \frac{k c^2}{a^2} - \frac{\Lambda c^2}{3} - \frac{8\pi G}{3 c^2} \rho = 0.$$  

(The second Friedmann equation is obtained by studying the equation of motion of $L_{\text{FRW}}$ together with the continuity equation, see details in [3, 12, 13].) As function of $\rho$ and $a$, the Hamiltonian reads:

$$H_{\text{FRW}} = -\frac{1}{4C} \frac{p^2}{a} + C \left(-\frac{k c^2}{a} + \frac{\Lambda c^2}{3} a^3 + \frac{8\pi G}{3c^2} \rho a^3\right)$$  

(7)

When promoting $H_{\text{FRW}}$ as an operator via $a \rightarrow a$ and $p \rightarrow -i\hbar \partial_a$ and by choosing the ordering $\frac{a^2}{\alpha} = \frac{1}{\alpha} \rho^2$ (the following results do not depend on this choice as we will explain later) one obtains the stationary Schrödinger equation with zero energy:

$$\left[-\hbar^2 \frac{d^2}{da^2} + V_{\text{eff}}(a)\right] \Psi(a) = 0$$

with

$$V_{\text{eff}}(a) = 4C^2 \left(k c^2 a^2 - \frac{\Lambda c^2}{3} a^4\right) - \frac{\alpha \hbar^2}{a^2}.$$  

(8)

This is the famous WDW equation. It is a timeless equation: a discussion about the emergence of time can be found in the literature [2, 17, 34, 35].

Here we are interested in the very early time evolution, therefore we consider $\rho = \rho_{\text{int-dom}} = A_{\text{int-dom}}/a^6$ (we neglect dust and radiation as well as other contributions, which become important at later stages of the evolution). Thus, our final form for the effective potential reads:

$$V_{\text{eff}}(a) = 4C^2 \left(k c^2 a^2 - \frac{\Lambda c^2}{3} a^4\right) - \frac{\alpha \hbar^2}{a^2}.$$  

(9)

The first term in the parenthesis is the one usually studied for the early quantum cosmology [7, 8, 11, 33], and the second piece represents the additional part being the main subject of the present work. It is parametrized by the dimensionless coupling $\alpha$

$$\alpha = 4C^2 \frac{8\pi G}{3c^2\hbar^2} A_{\text{int-dom}} = 6\pi^3 \frac{c^2}{G\hbar^2} A_{\text{int-dom}}.$$  

(10)

Thus, for $a$ very small, the term $-\alpha \hbar^2/\alpha^2$ dominates, leading to the WDW equation

$$\left[\frac{d^2}{da^2} + \frac{\alpha}{a^2}\right] \Psi(a) = 0 \quad \text{(for a very small)}.$$  

(11)

The potential $-1/a^2$ has very remarkable properties that have been studied in detail in Refs. [27, 29]. Since $\alpha$ in Eq. (10) is dimensionless, there is no typical energy scale in the problem: writing the eigenvalue equation for this potential, one can infer that –if it admits a bound state– there are infinite bound states, or in other terms there is no ground state. By indicating with $k_0^2$ the eigenvalue of the operator on the l.h.s. of Eq. (11) (which, in our case is set zero in order to recover the WDW equation of (11)), one can show that $\Psi(a) \propto \sqrt{a} K_i(g k_0 a)$, where $g = \sqrt{\alpha} - 1/4$ and $K_i$ is the modified Bessel function of order $i g$ [27]. Then, one concludes that the wave function $\Psi(a)$ vanishes in $a = 0$:

$$\Psi(a = 0) = 0.$$  

(12)

This is a first important and general result of our study: when considering an interaction dominated fluid that could have appeared just after the big bang, the wave function of the Universe fulfills the requirement postulated long ago by DeWitt to solve the problem of the big-bang singularity. A second properties of the $1/a^2$ attractive potential concerns a superselection rule imposed on the allowed range of the variable $a$. As shown in [28], the quantum system is confined to $a > 0$ (or $a < 0$) [28]; in other words, there is no linear superposition of wave functions which live at $a > 0$ with the ones at $a < 0$. Hence, there is no problem with negative values of $a$.

Next, we turn to explicit solutions in order to show that the wave function is real. When interpreting $H_{\text{FRW}}$ as an operator associated to a physical observable (i.e. the Hamiltonian) one has to verify that the operator is a self-adjoint operator i.e. it is symmetric and the domain of it coincides with the domain of its adjoint. As discussed in [27], the
property of self-adjointness for the $-1/a^2$ potential is obtained by imposing a specific boundary condition on the wave function (see Eq. (73) and (81) of Ref. [27], see also Ref. [30]). For $g = \sqrt{\alpha - 1/4} \neq 0$,

$$\sqrt{a} \left[ e^{2i g \log \frac{a}{a_0}} - 1 \right] \frac{d\Psi^*(a)}{da} - \frac{1}{\sqrt{a}} \left[ \left( \frac{1}{2} + ig \right) e^{2i g \log \frac{a}{a_0}} - \left( \frac{1}{2} + ig \right) \right] \Psi^*(a) \to 0 ,$$

(13)

while for $g = \sqrt{\alpha - 1/4} = 0$

$$\sqrt{a} \log \frac{a}{a_0} \frac{d\Psi(a)}{da} - \frac{1}{\sqrt{a}} \left[ 1 + \frac{1}{2} \log \frac{a}{a_0} \right] \Psi(a) \to 0 .$$

(14)

The general solution of Eq. (11) is a linear combination of two independent functions with, in general, complex coefficient. However, when imposing Eqs. (13) and (14) for the cases $g \neq 0$ and $g = 0$ respectively, one finds that only real wave functions are allowed. Let us discuss the case $g = 0$: the solution is $\Psi(a) = \sqrt{a}(c_1 + c_2 \log(a/a_0))$ where $c_1$, $c_2$ are complex numbers. Eq. (14) leads to the conditions $c_1 = 0$ and $c_2$ can be chosen as a real number, thus the wave function is real. Similarly, one can compute the solution in the general case $g \neq 0$: $\Psi(a) = \sqrt{ae^{-i\delta}}(c_1 + c_2x^{2i\theta})$ and impose the limit of Eq. (13). After a straightforward calculation, the solutions for the wave function very close to the big-bang can be recasted in the following compact form:

$$\Psi(a) = \begin{cases} 
N \sqrt{a} \sin \left[ g \ln(a/a_0) \right] & \text{for } g > 0 \text{ (i.e., } \alpha > 1/4) \\
N \sqrt{a} \ln(a/a_0) & \text{for } g = 0 \text{ (i.e., } \alpha = 1/4) \\
N \sqrt{a} \left[ (a/a_0)^{-g} - (a/a_0)^g \right] & \text{for } g = i\delta > 0 \text{ (0 < } \delta < 1/2, \text{ i.e. } 0 < \alpha < 1/4) 
\end{cases}$$

(15)

These solutions summarize the results of this paper. As anticipated previously, $\Psi(a = 0) = 0$: the wave function vanishes at the big-bang, thus offering a possible solution of the singularity problem (this is why $\alpha$ cannot be negative, otherwise $\Psi(a)$, although formally still given by the last line of Eq. (15), would be divergent for $a \to 0$). Moreover, we also have that $\Psi(a = a_0) = 0$, i.e., the wave function also vanishing at the length emerging via the process of anomalous breaking of dilatation symmetry. However, the value of the constant $a_0$ cannot be determined. At first, it seems natural to set $a_0 \simeq \sqrt{\frac{3G}{c^2}} = \ell_P \simeq 10^{-33} \text{ cm}$, but there is actually no compelling reason for that. The eventual role of this new fundamental length $a_0$ should be investigated in the future. The constant $N$ is a normalization constant which can be always taken as real, therefore $\Psi(a)$ is real. There is no problem for $a \to 0$, and also no problem for $a < 0$ (it never goes to $a < 0$ without imposing any additional requirement).

Finally, it is important to show that our main outcomes do not depend on the order of the operators. Other prescriptions induce a shift of the critical value of $\alpha$, but there is no qualitative change of our discussion. For instance, for the choice $\frac{\partial^2}{\partial a^2} \rightarrow \hat{p} \frac{1}{a^2} \hat{p}$ (as in [11]) one still finds that $\Psi(a \to 0) = 0$ for each $\alpha > 0$. Upon defining $\Psi_{new}(a) = \Psi(a)/\sqrt{a}$, Eq. (11) is re-obtained for a shifted $\alpha$:

$$\left[ \frac{d^2}{da^2} + \frac{\alpha_{new}}{a^2} \right] \Psi_{new}(a) = 0 ,$$

(16)

with $\alpha_{new} = \alpha - \frac{1}{4}$. Thus, being $\Psi_{new}(a)$ real, $\Psi(a)$ is also such. For the critical value $\alpha_{new} = 1/4$ (hence, $\alpha = 1$), $\Psi(a) = Na \ln(a/a_0)$. (For $\alpha < 3/4$, $\alpha_{new} < 0$, $\Psi_{new}(a)$ is still given as the last line of Eq. (15), but for $\delta > 1/2$, hence $\Psi_{new}(a \to 0)$ diverges. There is however no problem since this divergence is compensated by $\sqrt{a}$ as long as $\alpha > 0$. The wave function $\Psi(a)$ always vanishes at the big-bang for positive $\alpha$).

More in general, let us consider the two-parameter parametrization $\frac{d^3}{da^3} \rightarrow \frac{1}{a} \hat{p} \frac{1}{a^2} \hat{p} \frac{1}{a^2} \hat{p}$ \cite{36} (our case corresponds to $i = 1$, $j = 0$, Vilenkin’s choice to $i = 0$, $j = 1$, the parametrization $j = 1 - i$ was studied in Ref. \cite{37,38}). The very same steps can be performed. The wave function is such that $\Psi(a \to 0) = 0$ for any $\alpha > 0$ as long as $i \geq 0$, $j \geq 0$ and $i + j \leq 1$ (intuitively, we split $1/a$ into three parts, each one with a positive power in the denominator). A redefinition $\Psi_{new}(a) = a^{-\delta} \Psi(a)$ for which Eq. (16) holds for $\delta$ and $\alpha_{new}$ obtained by a straightforward calculation:

$$\alpha_{new} = \alpha + \frac{1}{4} - \frac{1}{4} \left( (3 - 2i - j)^2 - 4(i - 2)j \right) , \quad \delta = \frac{1 - 2i - j}{2} .$$

(17)

For the critical value obtained for $\alpha_{new} = 1/4$, one obtains $\Psi(a) = a^{-\frac{3-2i}{4}} \ln(a/a_0)$ where $\frac{3-2i-1}{4}$ is always positive in the chosen ranges for $i$ and $j$. Again, $\Psi_{new}(a)$ is real, then also $\Psi(a)$ is real.

A numerical example: For larger values of $a$, the terms proportional to $\Lambda$ and $k$ become important. It is then instructive to study a numerical case which is reminiscent of the potentials studies in Refs. \cite{7,8,11,33}, with the
inclusion of the additional short-range $-1/a^2$ potential. To this end, we start by rewriting the WDW equation in natural units and in terms of the dimensionless $a' = a/\sqrt{G}$:

\[- \frac{d^2\Psi}{da'^2} + V_{\text{eff}}(a')\Psi = 0 \text{ where } V_{\text{eff}}(a') = ka'^2 - \lambda a'^4 - \frac{\alpha}{a'^2}, \tag{18}\]

with dimensionless constants $k = \frac{2\pi^2}{k^4}$, $\lambda = \frac{3\pi^2}{4\Lambda^2}$, and $\alpha$ already introduced in Eq. (10). In general, we could not find analytic solutions of this equation and we did not derive the conditions of self-adjointness of this new operator. However, the behavior of the wave function close to $a' = 0$ should be anyway dominated by the $1/a'^2$ term and thus we will again have solutions which vanish in $a' = 0$ and are real, see Fig. 1 for an illustrative example.

It is easy to prove that the wave function is $L^2(0, +\infty)$: indeed in the limit $a' \to \infty$, Eq. (18) admits solution of the type $\sqrt{a'}\text{BesselJ}(\pm 1/6, \sqrt{\lambda a'^3}/3)$ which scales as $1/a'$ at infinity. We thus find a solution which interpolates between the analytical one in Eq. (15) and the one of Hartle and Hawking (real and normalizable).

Conclusions: In this work, we have studied the effect of a stiff matter component in the very early phase of the Universe. The corresponding potential in the WDW equation is proportional to $-1/a^2$. This very interesting and atypical potential has some remarkable features for the WDW equation: the wave function vanishes at the origin, is defined only for positive $a'$, and is real. Moreover, our qualitative results do not depend on a large class of choices of the operator ordering of the WDW equation. In the future, more detailed and more realistic numerical studies which take into account such an interaction dominated gas as well as additional terms are needed. The investigation of possible phenomenological implication of an initial stiff matter on the early inflation and on present cosmological observables represent a promising outlook of the present work.

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