Self-Adjoint Wheeler-DeWitt Operators, the Problem of Time and the Wave Function of the Universe

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Abstract

We discuss minisuperspace aspects a non empty Robertson-Walker universe containing scalar matter field. The requirement that the Wheeler-DeWitt (WDW) operator be self adjoint is a key ingredient in constructing the physical Hilbert space and has non-trivial cosmological implications since it is related with the problem of time in quantum cosmology. Namely, if time is parametrized by matter fields we find two types of domains for the self adjoint WDW operator: a non trivial domain is comprised of zero current (Hartle-Hawking type) wave functions and is parametrized by two new parameters, whereas the domain of a self adjoint WDW operator acting on tunneling (Vilenkin type) wave functions is a single ray. On the other hand, if time is parametrized by the scale factor both types of wave functions give rise to non trivial domains for the self adjoint WDW operators, and no new parameters appear in them.

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1 Introduction

One of the simplest models of quantum cosmology is the Robertson-Walker (RW) minisuperspace. RW geometries describe homogeneous and isotropic universes. The RW geometry is defined by the line element

\[ ds^2 = -N_\perp^2 d\eta^2 + a^2(\eta) d\Omega_3^2. \]  

(1.1)

In (1.1) the only dynamical degree of freedom is the scale factor \( a(\eta) \). The lapse function \( N_\perp \) is not dynamical, being a pure gauge variable. The quantity \( d\Omega_3^2 \) is the standard line element on the unit three-sphere. We use units in which \( \hbar = c = 1 \) and \( G = M_p^{-2} = 3\pi/4 \).

The pure gravitational action corresponding to (1.1) is

\[ S_g = \frac{1}{16\pi G} \int_M d^4x \sqrt{-g} (R - 2\Lambda) + \frac{1}{8\pi G} \int_{\partial M} d^3x \sqrt{g^{(3)}} K \]

\[ = \int d\eta N_\perp a^3 \left[ a^{-2} \left( 1 - \frac{\dot{a}^2}{N_\perp^2} \right) - \frac{\Lambda}{3} \right]. \]  

(1.2)

In (1.2) \( \Lambda \) is the cosmological constant\(^4\). \( M = I \times S^3 \) is the space-time manifold, \( K = K^i_i \) is the trace of the second fundamental form of the space-like boundary \( \partial M = S^3 \) (defined by \( \eta = \text{const.} \)) and the dot denotes differentiation with respect to \( \eta \). The Hamiltonian corresponding to (1.2) is

\[ H = -N_\perp \left( \frac{1}{4a} P_a^2 + a - g^2 a^3 \right) \]  

(1.3)

where \( P_a = \partial L/\partial \dot{a} = -2a \dot{a}/N_\perp \) is the canonical momentum conjugate to \( a(\eta) \) and \( g^2 = \frac{\Lambda}{3} \). It is assumed in (1.3) that \( \Lambda \geq 0 \). Gauge invariance of (1.2) yields the Hamiltonian constraint

\[ -\frac{\partial H}{\partial N_\perp} = \frac{1}{4a} P_a^2 + a - g^2 a^3 = 0. \]  

(1.4)

The constraint (1.4) requires a gauge fixing condition. A possible such gauge fixing condition is \( N_\perp = \text{const.} \neq 0 \) in which the time variable \( \eta \) becomes essentially the

\(^4\)One can regard \( \Lambda \) as a pure cosmological constant or as the vacuum energy of some non trivial field configurations, or a sum of both.
proper time \( \tau \). In this gauge the solution of the classical equations of motion (with initial conditions \( a(0) = g^{-1}, \dot{a}(0) = 0 \)) is

\[
a(\tau) = g^{-1} \cosh(g \tau),
\]

which describes a universe that contracts from an infinite radius in the absolute past, reaches a minimum radius, \( a_{\text{min}} = g^{-1} \), and re-expands to infinity in the absolute future.

Quantization of this simple system is accomplished straightforwardly in the coordinate representation by the usual operator realizations

\[
\hat{a} = a \quad \text{and} \quad \hat{P}_a = -i \frac{\partial}{\partial a}.
\]

Neglecting operator ordering problems in the kinetic term\(^2\) the Hamiltonian constraint becomes the Wheeler-DeWitt (WDW) equation \([1, 2]\) for the wave function of the Universe:

\[
\left( -\frac{1}{4a} \frac{\partial^2}{\partial a^2} + a - g^2 a^3 \right) \Psi(a) = 0.
\]

Equation (1.7) is a Schrödinger equation \( \hat{H} \Psi = 0 \) for a zero energy eigenstate of a mass \( m = 2 \) particle, moving in the one dimensional potential

\[
V(a) = a^2 - g^2 a^4.
\]

Despite the fact that the potential (1.8) is unbounded from below, it has the property that the time of flight of a classical particle from the largest turning point to infinity is finite, namely,

\[
\int_{x_0 > \frac{1}{g}}^{\infty} \frac{dx}{\sqrt{|V(x)|}} < \infty.
\]

This may seem contradictory to (1.5) at first sight, because this equation implies \( \tau \to \infty \) as \( a \to \infty \). However, this contradiction is only apparent, since what we call “time” in (1.9) is not the proper time \( \tau \). In order that the classical particle that

\(^2\)In this work we study only semiclassical solutions to the WDW equation, where operator ordering issues are not so important.
moves in the one dimensional potential $(1.8)$ have the standard kinetic energy term (that is an implicit assumption in $(1.9)$), one must impose the “conformal time” gauge $N_\perp = a(t)$ on $(1.3)$. Doing so, $(1.3)$ becomes

$$H = -\left(\frac{P^2_0}{4} + a^2 - g^2 a^4\right). \quad (1.10)$$

The functional relation between the conformal time and proper time is

$$t = \int \frac{d\tau}{a(\tau)} = \tan^{-1}\left(\sinh(g\tau)\right) \quad (1.11)$$

and the classical solution $(1.3)$ in the conformal gauge is

$$a(t) = \frac{1}{g\cos(t)}. \quad (1.12)$$

It is clear from $(1.12)$ that the “particle” reaches infinity indeed after finite conformal time, $t = \pi/2$.

Eq. $(1.9)$ suggests that one dimensional Schrödinger operators like $(1.10)$ are very similar to Schrödinger operators describing quantal systems defined on a finite segment of the real line, despite the fact that they act on wave functions supported along the real positive half line. Quantal systems defined on a finite segment require boundary conditions as an essential part of their definition. In a similar manner, Schrödinger operators like $(1.10)$ require boundary conditions on wave functions, ensuring probability conservation at infinity. Thus, such conditions extend ill defined Hamiltonians like $(1.10)$ into a self-adjoint form which generate unitary time evolution operators.

Considerations of extending the Hamiltonian $(1.10)$ into a self-adjoint form seem irrelevant for quantum cosmological considerations at first sight. Indeed, solutions of the WDW equation $(1.7)$ for the pure RW geometry $(1.1)$ are always the zero energy eigenstate of $(1.10)$ which spans a one dimensional Hilbert space on which $(1.10)$ is trivially self adjoint.\footnote{Note that the usual arguments that guarantee non-degeneracy of the discrete spectrum of one dimensional Schrödinger operators, and in particular that the corresponding wave function are real up to an overall phase, are inapplicable for the operator in $(1.10)$ which is unbounded from below. We elaborate on this point in section 3.} This is, however, only an incorrect superficial statement. There are at least two important reasons to introduce self-adjoint extensions
of the WDW Hamiltonian of which \((1.10)\) is only a very simple case. First, we note that the null condition \((1.4)\) is just a special case of the general constraint enforcing reparametrization invariance on physical states in quantum gravity, namely, that they be annihilated by the WDW operator. This implies that one has to consider the WDW operator defined in a Hilbert space larger than the space of physical states, where one can apply it on various states and check whether they are physical or not. In this framework of constrained quantization it is always assumed that all relevant operators, and in particular, the constraint operators, are self-adjoint with respect to the Hilbert space inner product\([8]\). In our particular case, this means that we have to include in the domain of definition of the operator \((1.10)\) many eigenstates with non vanishing energy eigenvalues. In this case, the issue of a proper self-adjoint extension of \((1.10)\) becomes important.

Second, note that when cases of a non-empty RW universes or perturbed RW universes \([9, 10]\) are considered, many non zero energy eigenstates of \((1.10)\) become relevant, even in the physical Hilbert subspace itself. This comes about because now the WDW constraint implies that the total Hamiltonian must annihilate physical states. To see this we observe that the total Hamiltonian may be written as

\[
H_{WDW} \equiv H_{tot} = H_{\phi,h_{\mu\nu}} - H_0 \tag{1.13}
\]

where \(-H_0\) is \((1.10)\) and \(H_{\phi,h_{\mu\nu}}\) is the Hamiltonian of matter fields (denoted here by the field \(\phi\)) and of gravitational perturbations (denoted by \(h_{\mu\nu}\))\([4]\). The minus sign in \((1.13)\) results from the fact that the kinetic term of the conformal mode \(a\) in \((1.2)\) appears with the “wrong” sign. In simple cases where a separation of variables applies, \(|\psi\rangle = |\phi_a\rangle|\chi_{\phi,h}\rangle\), the corresponding WDW equation reduces into the two equations

\[
\hat{H}_0|\phi_a\rangle = E|\phi_a\rangle \tag{1.14}
\]

and

\[
\hat{H}_{\phi,h}|\chi_{\phi,h}\rangle = E|\chi_{\phi,h}\rangle \tag{1.15}
\]

\(^4\)That is, the metric is \(g_{\mu\nu} = g_{\mu\nu}^{(0)} + h_{\mu\nu}\) where \(g^{(0)}\) is the RW metric in \((1.1)\).
where $E$ is some non-negative eigenvalue\footnote{The requirement that $E \geq 0$ is a consequence of the energy condition for matter fields.} either of $\hat{H}_0$ or of $\hat{H}_{\phi,h}$. Now, in principle, many eigenstates of $\hat{H}_0$ and of $\hat{H}_{\phi,h}$ (sharing the same eigenvalue) may enter into the quantum state of the Universe, especially if it turns out to be a quasi-classical state\footnote{A quasi-classical state is a superposition of many energy eigenstates which are superimposed with some well behaved amplitudes, for example,}

Now that many different energy eigenstates of (1.14) and (1.15) are used to construct physical states, one has to equip them with a *time independent* inner product in order to define the physical Hilbert space. We find that if we choose matter fields as our clock, self-adjointness of (1.10) turns out to be the necessary and sufficient condition for the existence of such an inner product. In this case there is a continuous two parameter family of non trivial domains of the self-adjoint WDW operator that are spanned by zero current (Hartle-Hawking type) wave functions, whereas the domain of a self adjoint WDW operator acting on tunneling (Vilenkin type) wave function is trivially a single ray. One can define a positive definite Hilbert space inner product using both kinds of wave functions. If, on the other hand, we choose the scale factor of the Universe to parametrize time, both wave functions give rise to non trivial domains, and are independent of any new parameters. However, positive norm physical states may be constructed using only Vilenkin type wave functions. Therefore, whenever we are free to choose either matter fields or the scale factor as a time coordinate, self-adjointness of the (spatial part of the) WDW operator dictates utterly different physical Hilbert spaces corresponding to different physical realities, and is therefore intimately related to the problem of time in quantum gravity\cite{12}.

In section 2 we consider a non-empty RW universe filled up with matter in the form of scalar fields where we derive (1.13)-(1.15) explicitly. We show how the requirement for self-adjointness of the (spatial part of the) WDW operator arises and point its relation to the problem of time. In section 3 we discuss self-adjoint extensions of one
dimensional Schrödinger operators whose potential terms are unbounded from below, but satisfy (1.9). In section 4 we apply such extensions to RW quantum cosmology and discuss the Hartle-Hawking and Vilenkin proposals for the wave function of the Universe in this context. Finally, we show in the appendix that the domain of the self adjoint WDW operator (1.10) acting on tunneling (Vilenkin type) wave functions is a single ray.
Consider a scalar field $\phi(\eta, \vec{x})$ which is coupled non-minimally to gravity. It is governed by the action

$$S_m = -\frac{1}{2} \int_M d^4x \sqrt{-g} \left[ \partial_\mu \phi \partial^\mu \phi + \xi R \phi^2 + V(\phi) \right] - \frac{1}{2} \xi \int_{\partial M} d^3x \sqrt{g^{(3)}} K \phi^2. \quad (2.1)$$

where $\xi$ is the coupling constant. In the homogeneous and isotropic case, we have $\phi = \phi(\eta)$, and thus the total action (namely, the sum of (1.2) and (2.1)) is

$$S_{tot} = S_g + S_m = \int d\eta N_\perp \left[ -a \frac{\dot{a}^2}{N^2_\perp} + a^3 - 12 \xi a^2 + U(a, \chi) \right] \quad (2.2)$$

where $\chi \equiv \pi a^{6\xi} \phi$ is the rescaled matter field and

$$U(a, \chi) = a - g^2 a^3 - \pi^2 a^3 V\left(\frac{\chi}{\pi a^{6\xi}}\right) - 6 \xi a^{1-12\xi} \chi^2. \quad (2.3)$$

The corresponding Hamiltonian is

$$H_{WDW} \equiv H_{tot} = N_\perp \left[ -\frac{1}{4a} P_a^2 + \frac{1}{4a^{3-12\xi}} P_\chi^2 - U(a, \chi) \right]. \quad (2.4)$$

In the coordinate representation $\hat{P}_a = -i \frac{\partial}{\partial a}$ and $\hat{P}_\chi = -i \frac{\partial}{\partial \chi}$, the WDW equation reads

$$\left[ -\frac{1}{4} \frac{\partial^2}{\partial a^2} + \frac{1}{4} a^{12\xi-2} \frac{\partial^2}{\partial \chi^2} + a U(a, \chi) \right] \Psi(a, \chi) = 0. \quad (2.5)$$

We concentrate on the simple conformally invariant case where $V(\phi) = 0$ and $\xi = 1/6$, such that (2.4) becomes

$$H_{WDW} \equiv H_{tot} = -\frac{N_\perp}{a} \left( \frac{1}{4} P_a^2 - \frac{1}{4} P_\chi^2 + a^2 - g^2 a^4 - \chi^2 \right). \quad (2.6)$$

The WDW equation is therefore

$$\left( -\frac{1}{4} \frac{\partial^2}{\partial a^2} + a^2 - g^2 a^4 + \frac{1}{4} \frac{\partial^2}{\partial \chi^2} - \chi^2 \right) \Psi(a, \chi) = 0. \quad (2.7)$$

We solve (2.7) by separation of variables $\Psi(a, \chi) = \psi_a(a) \psi_\chi(\chi)$, which results in the two coupled equations

$$\left( -\frac{1}{4} \frac{\partial^2}{\partial a^2} + a^2 - g^2 a^4 \right) \psi_a(a) = E \psi_a(a) \quad (2.8)$$

$$\left( -\frac{1}{4} \frac{\partial^2}{\partial \chi^2} + \chi^2 \right) \psi_\chi(\chi) = E \psi_\chi(\chi). \quad (2.9)$$
Quantization requires gauge fixing, namely a definition of “time”. The freedom left in making such a gauge choice leads to the “problem of time” in quantum cosmology [12, 13]. It is strongly related to the definition of a physical Hilbert space, and here is the place where considerations of self-adjointness come into play [14]. One has to introduce an inner product in the space of solutions to the WDW equation (2.7) in order to define the physical Hilbert space. Defining the currents $J^{12}_{a,\chi} = i\Psi^*_1 \hat{\partial}_{a,\chi} \Psi_2$, we have

$$\partial_a J^{12}_{a,\chi} - \partial_\chi J^{12}_{\chi} = 0.$$ (2.10)

for any pair $\Psi_1, \Psi_2$ of solutions of (2.7).

In our simple minisuperspace model we can choose the time variable either as the scale factor $a$ or as the matter field $\chi$ [14, 15, 16]. If we choose the scale factor $a$ as our time, $t = a$, then

$$\langle \Psi_1 | \Psi_2 \rangle_{(a)} = -i \int_{-\infty}^{\infty} d\chi \left[ \Psi^*_1(a,\chi) \hat{\partial}_a \Psi_2(a,\chi) \right]_{|a=t=const.}$$ (2.11)

is a natural inner product to use in constructing the physical Hilbert space.

A well defined inner product among solutions of (2.7) is necessarily time independent in order that there be no conflict between time evolution of physical states and the definition of Hilbert space at each time slice $t = \text{constant}$. Deriving (2.11) with respect to time we have

$$i\partial_t \langle \Psi_1 | \Psi_2 \rangle_{(a)} \equiv i\partial_t \langle \Psi_1 | \Psi_2 \rangle_{(a)} = J^{12}_{\chi}(+\infty) - J^{12}_{\chi}(-\infty),$$ (2.12)

where we have used (2.10) and integrated over $\chi$. Therefore, time independence of (2.11) implies

$$J^{12}_{\chi}(+\infty) - J^{12}_{\chi}(-\infty) = 0.$$ (2.13)

This condition holds automatically due to finiteness of (2.11) which also leads to a discrete spectrum of (2.9). The latter is the standard one dimensional harmonic oscillator spectrum, $E_n = \omega(n + 1/2) = (n + 1/2)$, for which $J^{12}_\chi(+\infty) = J^{12}_\chi(-\infty) = 0$

7 The discussion in [14] is limited to the case of zero cosmological constant for which there is no need for self adjoint extensions of the WDW operator.
The Schrödinger operator on the left hand side of (2.9) which is the spatial part of the WDW operator in (2.6) is clearly self-adjoint in this domain. Evidently, (2.13) sets no restrictions on the Schrödinger operator on the left hand side of (2.8) and therefore self-adjointness of the WDW operator leads to no further consequences in this case. This implies, as we show in the next two sections, that a non trivial domain of the self-adjoint WDW operator includes either zero-current (zero-norm) wave functions or tunneling wave functions.

Matters are utterly different when we choose \( \chi \) (and not \( a \)) as time. In this event, the roles of \( \chi \) and \( a \) interchange. One should integrate (2.10) over \( a \), and the inner product is therefore

\[
\langle \Psi_1 | \Psi_2 \rangle_{(\chi)} = -i \int_0^\infty da \left[ \Psi_1^* (a, \chi) \frac{\partial}{\partial \chi} \Psi_2 (a, \chi) \right]_{\chi=t=\text{const.}}. 
\]

This inner product is time independent (\( \chi \) independent) only if

\[
J_a^{12} (+\infty) - J_a^{12} (0) = 0 \quad (2.15)
\]

for any pair of solutions \( \Psi_{1,2} \) of (2.7). This condition is quite different from (2.13). Unlike the latter, it is not satisfied automatically, because the potential energy in (2.8) is unbounded from below. Rather, it must be imposed, in order that the Schrödinger operator on the left hand side of (2.8) which is the spatial part of the WDW operator in (2.4) for this choice of time parametrization, be well defined. Indeed, (2.13) is precisely the condition that the Hamiltonian on the left hand side of (2.8) be symmetric with respect to this inner product. This can be accomplished by defining proper self-adjoint extensions of the Hamiltonian as we discuss in the next two sections. Namely, we show there that (2.15) implies that zero current wave functions (similar in form to the Hartle-Hawking wave function) give rise to a two parameter continuous family of non trivial domains for the self adjoint WDW operator whose spectrum \( \{E_n\} \) is discrete and highly non linear in \( n \). On the other hand, the domain of a self adjoint WDW operator acting on tunneling (Vilenkin type) wave functions is a single ray having a single eigenvalue.
Demanding that the Hamiltonian be self-adjoint is equivalent to the requirement of unique time evolution of quantum states. We see that the two different choices of “time” in this model lead to different kinds of physical Hilbert spaces and therefore to two highly different physical “realities”. Thus, the requirement that the spatial part of the WDW operator be self-adjoint is intimately related with the problem of time in in quantum cosmology which manifests itself to its extreme in the model discussed here.

We are not going to argue here which choice of time coordinate is superior to the other. However, we feel that the choice \( t = \chi \) has not received enough attention (at least as far as mathematical aspects are concerned), and we wish to fill this gap partially. On top of this, note that implications of self-adjointness of the (spatial part of the) WDW operator are less trivial here compared to those related with the other possible choice.

In the non conformally invariant case, the WDW equation is generally non-separable and therefore much more complicated. However, in cases where \( V(\chi) \) has a narrow deep minimum at \( \chi = \chi_s \) we can assume to a first approximation that \( \chi \) does not fluctuate far away from that minimum and thus replace \( V(\chi) \) by its minimal value \( \rho_s = V(\chi_s) \). In this approximation one thus merely shifts \( g^2 \) into \( g_{\text{eff}}^2 = g^2 + \pi^2 \rho_s \).

We close this section making some general remarks before turning to the formal discussion of the proper self-adjoint extensions of (2.8). Strictly speaking, the scale factor \( a \) in (1.1) is defined on the ray \( a \geq 0 \). Therefore all Schrödinger operators involving \( a \) must be equipped with a suitable boundary condition at \( a = 0 \) in order to make them self-adjoint. Such a boundary condition is a necessary datum purely from the Schrödinger theory point of view and for this reason we will impose such a condition on wave functions below. However, which boundary condition at \( a = 0 \) must be imposed on (1.10) and (2.8) in order to describe quantum cosmology is a highly controversial issue. Indeed, unlike its usefulness at large radii, the mini-superspace formalism we use in this paper might break completely at extremely small radii of the Universe because of the true singularity of (1.4) at the point \( a = 0 \).
Should this happen, (1.10) and (2.8) will become useless at $a \to 0$ as well as their solutions. The region $a \gg 1/g$, on the other hand, is certainly in the validity domain of the minisuperspace quantization scheme. We may thus trust the wave functions resulting from the WDW equation only for large universe radii, as far as cosmological interpretations are concerned.

As was discussed in the introduction, the fact that the time of flight (1.9) of a classical particle moving in the potential (1.8) to infinity is finite has a very important consequence. Namely, it effectively turns the spectral problem involving the hamiltonian on the left hand side of (1.10) into a problem defined on a finite segment, despite the fact that $0 \leq a < \infty$. This calls for an appropriate boundary condition on wave functions at $a = \infty$ as well. The boundary condition imposed at $a = 0$ must be consistent with the one set at $a = \infty$. Thus, in principle, there is some influence by the $a = 0$ endpoint (where the minisuperspace formalism is suspicious) on the asymptotic behavior of the wave function of the Universe as $a \to \infty$ (where the minisuperspace formalism is surely valid). We comment on this point in section 4.
3 Domain of the Self-Adjoint Hamiltonian Defined on the Ray $0 \leq x < \infty$

Consider a particle of mass $m$, moving in the one dimensional potential

$$V(x) = x^2 - g^2 x^4, \quad x \geq 0$$

(3.1)

having energy $0 \leq E \leq \frac{1}{4g^2}$. There are two classically allowed regions for this range of energies, $x \leq x_1$ and $x \geq x_2$. Here $x_2(E) > x_1(E) > 0$ are the two classical turning points, namely, the two positive real roots of $V(x) = E$.

A wave packet with energy distribution peaked at $E$ will move in (3.1) from $x_i \geq x_2$ to infinity in a finite period of time

$$t_E = \int_{x_i}^{\infty} \frac{dx}{\sqrt{2m[E - V(x)]}},$$

(3.2)

raising the question what will happen to the wave packet as it “hits” the point at infinity or equivalently, how is probability conserved in such a system. Therefore, on account of (3.2), unbounded motion in the potential (3.1) behaves in many respects as if it were bounded, and the point at infinity appears as if it were the end point of a finite segment [7].

Probability conservation requires that the Hamiltonian governing this system be self-adjoint. This requirement on the domain of definition of the Hamiltonian is by no means trivial, since wave functions in the potential (3.1) have only power-like decay while their first derivatives blow up at infinity, as can be most easily seen by writing down the leading WKB approximation

$$\Psi_E(x) \sim \frac{1}{[E - V(x)]^{\frac{1}{4}}} \left\{ C_1(E) \sin \left[ \int_{x_2}^{x} \sqrt{2m(E - V(y))}dy - \frac{\pi}{4} \right] + C_2(E) \cos \left[ \int_{x_2}^{x} \sqrt{2m(E - V(y))}dy - \frac{\pi}{4} \right] \right\}$$

(3.3)

to a generic solution of the Schrödinger equation

$$\left[ -\frac{1}{2m} \frac{d^2}{dx^2} + V(x) \right] \Psi_E(x) = E \Psi_E(x)$$

(3.4)
in region \( x > x_2 \). Finiteness of \( t_E \) in (3.2) means that (3.3) is square integrable for any value of \( E \), but this is not true of its first derivative. Due to the fact that \( V(x \to \infty) \to -\infty \), local De-Broglie wave lengths of the particle become extremely short very quickly as it moves deeper into the classically allowed region rendering the WKB approximation more and more accurate as \( x \to \infty \) \(^8\). It is therefore enough to limit our discussion to the framework of the WKB approximation\(^7\). Such asymptotic behavior of \( \Psi(x) \) and \( \Psi'(x) \) as \( x \to \infty \) is in clear contrast with the exponential fall off of both bound state wave functions and their first derivatives in case of potentials that are bounded from below. In particular, it implies that there can be two square integrable linearly independent solutions of (3.4) sharing the same parameter \( E \) because their constant Wronskian need not vanish. Thus, square integrability is not sufficient to determine the spectrum, and what is needed is an explicit boundary condition at infinity which should be treated as if it were really a finite boundary point.

For any two states \( \Psi_1 \) and \( \Psi_2 \) in the domain of the self-adjoint Hamiltonian we must have

\[
\langle \hat{H} \Psi_1 | \Psi_2 \rangle = \langle \Psi_1 | \hat{H} \Psi_2 \rangle .
\] (3.5)

Using the coordinate representation and integrating by parts, (3.3) implies

\[
\left[ \frac{d}{dx} \Psi_1^* \Psi_2 - \Psi_1^* \frac{d}{dx} \Psi_2 \right]_0^+ = 0.
\] (3.6)

This is precisely the consistency condition (2.15) encountered above.

Considering non trivial domains of the self adjoint operator \( \hat{H} \), the current \( J^{12} = \frac{i}{2} (\Psi_2 \partial_x \Psi_1^* - \Psi_1 \partial_x \Psi_2) \) must vanish at the two boundary points, since otherwise a particle reaching \( x = \infty \) will have to reappear at \( x = 0 \) or vice versa. While such a periodic boundary condition is relevant for quantization of a particle in a finite rigid box\(^6\), it is clearly improper here because in our case \( V(0) = 0 \) while \( V(\infty) = -\infty \). We back this qualitative argument by an explicit calculation presented in the appendix.

\(^8\)Recall that this is also the region of scale factor \( a = x \) values where minisuperspace analysis is most valid anyway.
where we show that if the current \( J^{12} \) did not vanish, the domain of the self adjoint operator \( \hat{H} \) becomes trivial and collapses into a single ray.

Therefore, studying non trivial domains, (3.6) may be replaced by the stronger condition

\[
\left[ \frac{d\Psi_1^*}{dx} \Psi_2 - \Psi_1^* \frac{d\Psi_2}{dx} \right] (x \to \infty) = \left[ \frac{d\Psi_1^*}{dx} \Psi_2 - \Psi_1^* \frac{d\Psi_2}{dx} \right] (x = 0) = 0. \tag{3.7}
\]

We show now that (3.7) will not hold (at \( x \to \infty \)) for generic \( \Psi_1 = \Psi_{E_1} \) and \( \Psi_2 = \Psi_{E_2}; \ E_1 \neq E_2, \) unless some special choice of the functions \( C_1(E) \) and \( C_2(E) \) in (3.3) is made. To make this point clearer, it is useful to introduce the phase \( \phi_\alpha(E) \) defined by

\[
\cot (\phi_\alpha(E)) = -\frac{C_2(E)}{C_1(E)} \tag{3.8}
\]

where \( \alpha \) is a parameter wave functions depend upon and will be determined later. In terms of \( \phi_\alpha(E) \), (3.3) becomes

\[
\Psi_{E_\alpha}(x > x_2) \sim -\frac{C_1(E)}{[E - V(x)]^{1/4}} \sin \phi_\alpha(E) \cos \left[ \int_{x_2(E)}^x \sqrt{2m(E - V(y))} dy + \phi_\alpha(E) - \frac{\pi}{4} \right]. \tag{3.9}
\]

The cosine in (3.9) oscillates very rapidly as \( x \to \infty \) and therefore (3.7) will not be met (for \( E_1 \neq E_2 \)) unless the argument of the cosine becomes independent of \( E \) as \( x \to \infty \), namely,

\[
\frac{\partial}{\partial E} \left[ \int_{x_2(E)}^x \sqrt{2m(E - V(y))} dy + \phi_\alpha(E) \right] = 0, \quad x \to \infty. \tag{3.10}
\]

In order to solve (3.10) we need to specify an initial condition in \( E \), this is how the parameter \( \alpha \) gets in. One can choose

\[
\phi_\alpha(E = \alpha) = 0 \tag{3.11}
\]

and the solution of (3.10) (subjected to (3.11)) is

\[
\phi_\alpha(E) = \sqrt{2m} \left\{ -\int_{x_2(E)}^\infty \left[ \sqrt{E - V(y) - \sqrt{\alpha - V(y)}} \right] dy + \int_{x_2(\alpha)}^{x_2(E)} \sqrt{\alpha - V(y)} dy \right\}. \tag{3.12}
\]
where \( x_2(\alpha) \) is the largest root of \( V(x) = \alpha \). Substituting the specific potential (3.1) into (3.10) and integrating over \( E \) we obtain

\[
\phi_{\alpha}(E) = \begin{cases} 
\frac{1}{g^2} \int_{z(\alpha)}^{z(E)} \zeta^2 K(\frac{\zeta^2 - 1}{2\zeta^2}) d\zeta & ; \quad E \leq 0 \\
\frac{1}{g^2} \left[ C_\alpha + \int_{z(\alpha)}^{z(E)} \frac{\sqrt{2\zeta}}{\sqrt{1+\zeta^2}} K(\frac{1-\zeta^2}{1+\zeta^2}) d\zeta \right] & ; \quad E \geq 0
\end{cases}
\]

(3.13)

where \( z(E) = (1 - 4Eg^2)^{\frac{1}{4}} \), \( C_\alpha = \int_{z(\alpha)}^{z(E)} \zeta^2 K(\frac{\zeta^2 - 1}{2\zeta^2}) d\zeta \) and \( K(m) (E(m)) \) is a complete elliptic integral of the first (second) kind (we use \( E(m) \) below). Here we have also assumed \( \alpha < 0 \) so that \( C_\alpha < 0 \) as well.

From (3.12) we see that for \( x \to \infty \) (3.9) approaches

\[
\Psi_E^{(\alpha)}(x \to \infty) = -\frac{C_1}{[E - V(x)]^{\frac{1}{4}} \sin \phi_{\alpha}(E)} \cos \left[ \int_{x_2(\alpha)}^{x} \sqrt{2m(E - V(y))} dy - \frac{\pi}{4} \right]
\]

(3.14)

where the argument of the cosine is indeed \( E \) independent. It is clear now that (3.7) will hold at \( x \to \infty \) for any pair of functions \( \Psi_E^{(\alpha)} \), \( \Psi_E^{(\alpha)} \) of the form given by (3.9) and (3.12). These functions form a family of solutions of the Schrödinger equation (3.4) parametrized by the single (real) parameter \( \alpha \). These are not \textit{eigenstates} of the Hamiltonian, as we have not imposed (3.7) at \( x = 0 \) yet. To this end we note that a necessary and a sufficient condition for vanishing of the probability current at \( x = 0 \) is

\[
\frac{\Psi_E(x = 0)}{\Psi_E(x = 0)} = \beta
\]

(3.15)

where \( \beta \) is a fixed real number[3, 4, 5, 6].

In a similar manner to (3.9) we write the WKB solution of (3.4) as

\[
\Psi_E^{(\beta)}(x < x_1) = \frac{C_3(E)}{[E - V(x)]^{\frac{1}{4}} \sin \xi_{\beta}(E)} \cos \left[ \int_{x}^{x_1(E)} \sqrt{2m(E - V(y))} dy + \xi_{\beta}(E) \right]
\]

(3.16)

and (3.15) fixes

\[
\xi_{\beta}(E) = \arctan \left( \frac{\beta}{\sqrt{2mE}} \right) - \int_{0}^{x_1(E)} \sqrt{2m(E - V(y))} dy
\]

(3.17)
Eigenstates of (3.4) are obtained by matching (3.9) (subjected to (3.12)) and (3.16)-(3.17). Using the ordinary WKB matching conditions we obtain the corresponding “Bohr-Sommerfeld” quantization condition on $E$, namely,

$$4 \tan \phi_\alpha(E) = e^{-2\Delta(E)} \tan \left[ \frac{\pi}{4} - \xi_\beta(E) \right],$$

where

$$\Delta(E) = \int_{x_1(E)}^{x_2(E)} \sqrt{2m|E - V(y)|} dy$$

$$= \frac{\sqrt{2mx_2(E)}}{3g} \left[ \mathcal{E} \left( 1 - \frac{x_1(E)^2}{x_2(E)^2} \right) - 2g^2 x_1^2(E) \mathcal{K} \left( 1 - \frac{x_1(E)^2}{x_2(E)^2} \right) \right].$$

(3.18)

So far we have concentrated on energy range $0 \leq E \leq \frac{1}{4g^2}$. Our discussion may be extended in a straightforward manner to the complementary energy ranges $E > \frac{1}{4g^2}$ and $E \leq 0$ as well. For example, the quantization condition corresponding to $E > \frac{1}{4g^2}$ reads

$$\tan \left( \int_0^{\infty} \left( \sqrt{2m(E - V(y))} - \sqrt{2m(\alpha - V(y))} \right) dy \right) = - \frac{\beta}{\sqrt{2mE}}.$$

(3.20)

Note the explicit dependence of energy eigenvalues and eigenfunctions upon $\alpha$ and $\beta$. The spectrum is therefore a two parameter family $\{\Psi_E^{(\alpha,\beta)}(x)\}$, parametrized by $\alpha$ and $\beta$ as it should be in this case of separated boundary conditions according to the general theory of self-adjoint extensions [3, 4, 5, 6]. Due to (3.2) the point at infinity appears as if it were a finite endpoint and the whole quantum system behaves as if it were defined on a finite segment, where $\alpha$ and $\beta$ parametrize boundary conditions at the two endpoints. The set of functions $\{\Psi_E^{(\alpha,\beta)}(x)\}$ spans the domain of the self-adjoint Hamiltonian, namely, the space of all square integrable functions that satisfy (3.7).

Note that the WKB density of states

$$\rho_{WKB}(E) = \frac{m}{\pi} \int_0^{\infty} dx \frac{\theta[E - V(x)]}{\sqrt{2m[E - V(x)]}}$$

(3.21)
which is proportional to (3.2) is finite (as long as \( E \neq \frac{1}{4g^2} \)). The spectrum must be therefore discrete for \( \text{any} \ E \neq \frac{1}{4g^2} \) (with an accumulation point at \( \frac{1}{4g^2} \)). It is moreover bounded neither from below, nor from above and contains therefore an infinite amount of discrete states. Thus, the domain \( D^{\alpha,\beta} \) of the self-adjoint Hamiltonian is the set of all discrete linear combinations of the form

\[
\Psi^{(\alpha,\beta)}(x) = \sum_n c_n \Psi^{(\alpha,\beta)}_{E_n}(x),
\]

where \( \sum_n |c_n|^2 < \infty \) which yields an infinite dimensional Hilbert space.

\(^{9}\text{For} \ E \rightarrow \frac{1}{4g^2} \text{ (3.21) diverges logarithmically in } |E - \frac{1}{4g^2}|.\)
4 Quantum Cosmological Implications

The most important observation made in section 2 (as far as the simple cosmological model discussed there is concerned) is that time independence of the inner product in the definition of the physical Hilbert space leads to the requirement that the spatial part of the WDW operator, which is a one dimensional Schrödinger operator, be self adjoint. We saw in that section that one can choose time parametrization either in terms of the matter field $\chi$ or in terms of the scale factor $a$ of the Universe and that these two choices of time parametrization lead to different physical realities. In our view this is an extreme manifestation of the problem of time in quantum cosmology.

Our discussion in the previous two sections makes it clear that one may trace this discrepancy of physical realities to the fact that the two choices of time parametrization lead to two utterly different physical Hilbert spaces. The reason for this difference stems directly from the requirement that the (spatial part of the) WDW operator be self-adjoint. In this section we sharpen this distinction and investigate its cosmological implications in more detail.

Let us first concentrate on parametrization of time in terms of the scale factor $a$. From the discussion following (2.11) it is clear that a generic physical state has the form

$$\Psi(a, \chi) = \sum_{n \geq 0} c_n \psi_{an}(a) \psi_{\chi n}(\chi)$$

(4.1)

where $c_n$ are complex constants, $\psi_{\chi n}(\chi)$ is the normalized harmonic oscillator eigenstate corresponding to eigenvalue $E_n = (n + \frac{1}{2})$ and $\psi_{an}(a)$ is a normalized solution of (2.8) with parameter $E = E_n$ so that matter excitations are seemingly those of a free field. Because of orthonormality of the $\psi_{\chi n}(\chi)$ the inner product (2.11) of any two such states is simply

$$\langle \Psi^{(1)} | \Psi^{(2)} \rangle_{(a)} = \sum_{n \geq 0} j_n c_n^{(2)^*} c_n^{(1)}$$

(4.2)

Recall from our discussion in section 3 that these solutions are normalizable because of the finiteness of (3.3), as long as $E \neq \frac{1}{4\sqrt{g}}$. 

10
where \( j_n = -i[\psi^*_n(a)\psi_n(a)' - \psi^*_n(a)'\psi_n(a)] \) is the “Schrödinger” current carried by \( \psi_n(a) \). This current is clearly \( a \) independent, making (4.2) time independent in accordance with (2.12). The “Schrödinger” current carried by \( \psi_n(a) \) must be positive in order that (4.2) be positive definite. This positivity condition becomes simply

\[
|B_1(E)|^2 - |B_2(E)|^2 > 0
\]

(4.3)

where \( B_1 \) and \( B_2 \) are the amplitudes of the outgoing and of the incoming waves in the generic solution of (2.8) to the right of the largest turning point \( a_2 (V(a_2) = 0) \).

\[
\psi_{aE}(a > a_2) = \frac{1}{[E-V(a)]^{\frac{3}{4}}} \left\{ B_1(E) \exp \left[ i \int_{a_2(E)}^{a} \sqrt{4(E-V(y))} dy \right] + B_2(E) \exp \left[ -i \int_{a_2(E)}^{a} \sqrt{4(E-V(y))} dy \right] \right\} .
\]

(4.4)

For \( B_2 = 0 \), (4.4) gives pure expansion modes of the metric. The lowest mode (corresponding to \( n = 0 \)) is the original wave function suggested by Vilenkin[18]. Wave functions of the form (4.4) subjected to (4.3) may be referred to as “generalized tunneling wave functions” [10]. Note further that if we have \(|B_1(E)| = |B_2(E)|\) for all \( \psi_n(a) \) in (4.4) the latter describes standing wave modes of the form

\[
\psi_{aE}(a > a_2) = \frac{B(E)}{[E-V(a)]^{\frac{1}{4}}} \left\{ \cos \left[ \int_{a_2(E)}^{a} \sqrt{4(E-V(y))} dy + \phi(E) - \frac{\pi}{4} \right] \right\}
\]

(4.5)

carrying no current, that is \( j_n = 0 \) for all \( n \). The lowest of these modes \((n = 0, \phi(E) = 0)\) is the wave function suggested by Hartle and Hawking[19, 20, 11]. Following (4.2) one cannot associate probabilistic interpretation with such wave functions because all physical states in (4.1) become zero norm states.

We turn now to the case where time is parametrized by the matter field \( \chi = \pi a \phi \). Here the spatial part of the WDW operator is the Schrödinger operator in (2.8), which requires non-trivial self-adjoint extensions as we saw in the previous section.

It is shown in the appendix that in this case the domain of the self adjoint WDW

11Recall that here \( E = E_n > 0 \). For all practical uses we assume further that \( E < \frac{1}{\xi^2} \) so that \( a_2 > 0 \).
operator acting on tunneling (Vilenkin type) wave functions is trivial, namely, a single ray and the spectrum shrinks to a single point \( E = E_0 \). It is very interesting that the seemingly innocent requirement that the WDW operator be self adjoint is so powerful that it allows only a single physical state to exist. We stress that such a trivial domain occurs only for tunneling type wave functions. This may have the far reaching cosmological implication as the mechanism that selects the unique wave function of the Universe\(^{12}\).

The zero current wave functions span non-trivial domains of this self adjoint WDW operator. In the classically allowed region \( a > a_2 \) (which is the region where the minisuperspace approach is most reliable in the first place) the WKB approximation to the eigenfunctions spanning the non trivial domain are found from (3.9) as

\[
\psi_{an}^{(\alpha,\beta)}(a > a_2) = \frac{C(E_n)}{[E_n - V(x)]^{1/4}} \left\{ \cos \left[ \int_{a_2(E_n)}^a \sqrt{4(E - V(y))}dy + \phi_\alpha(E_n) - \frac{\pi}{4} \right] \right\}
\]

(4.6)

where \( \phi_\alpha(E) \) is given by (3.12) and \( E_n \equiv E_n^{(\alpha,\beta)} \) are solutions of (3.18). The modes given by (4.6) that appear in physical cosmological states must have non-negative energies \( E_n \geq 0 \) otherwise the energy condition for matter fields will be violated. We note here that for most practical purposes only energies in the range \( 0 \leq E_n \leq \frac{1}{4g^2} \) are important.

Clearly there is a continuous family of such domains parametrized by the two real continuous variables \( \alpha \) and \( \beta \). The functions (4.6) are standing wave modes of the geometry which are similar in form to the Hartle-Hawking wave function, but do not correspond to the “no-boundary” proposal for \( E > 0 \).

A generic physical state (corresponding to time parametrization by the matter field \( \chi = \pi a \phi \)) has the form

\[
\Psi^{(\alpha,\beta)}(a, \chi) = \sum_{n \geq 0} \psi_{an}^{(\alpha,\beta)}(a) \psi_{\chi n}(\chi)
\]

(4.7)

where now \( \psi_{\chi n}(\chi) \) are solutions of (2.9) with parameter \( E = E_n \). The functions

\(^{12}\)Note that the requirement of self adjointness by it self cannot fix \( E_0 \) which will hopefully be determined by the exact short distance Hamiltonian of quantum gravity.
\( \psi_{\chi n}(\chi) \) are therefore generic parabolic cylinder functions\[17, 21\] rather than harmonic oscillator eigenstates because the \( \{E_n\} \) in (3.18) are obviously not harmonic oscillator eigenvalues. It is convenient to express the general solution of the parabolic cylinder equation (2.9) in terms of the two linearly independent functions \( U_n \) and \( V_n \) as\[17\]

\[
\psi_{\chi n}(\chi) = b_n U_n(2\chi) + c_n V_n(2\chi),
\]

where

\[
U_n(z) = D_{E_n - \frac{1}{2}}(z) \quad \text{and}
\]

\[
V_n(z) = \frac{\Gamma(\frac{1}{2} - E_n)}{\pi} \left[ D_{E_n - \frac{1}{2}}(-z) - \sin(\pi E_n)D_{E_n - \frac{1}{2}}(z) \right].
\]

Here \( D_{\lambda}(z) \) are Whittaker functions, and \( \{b_n, c_n\} \) are complex constants.

The asymptotic behavior of the particular combinations of Whittaker functions appearing in (4.9) as \( z \to \pm \infty \) is\[17, 21\] \( U(z) \sim e^{\mp z^2/2}|z|^{\pm E - \frac{1}{2}} \) and \( V(z) \sim e^{\mp z^2}|z|^{\mp E - \frac{1}{2}} \), and their Wronskian is \( \sqrt{\frac{2}{\pi}} \).

Because of orthonormality of the \( \psi_{\alpha,\beta}^{(\alpha,\beta)}(\alpha) \) the (\( \chi \) independent) inner product (2.14) of any two states of the form (4.7) becomes

\[
\langle \Psi^{(1)}|\Psi^{(2)} \rangle_{(\chi)} = -i \sqrt{\frac{8}{\pi}} \sum_{n \geq 0} (b_n^{(1)*}c_n^{(2)} - c_n^{(1)*}b_n^{(2)}).
\]

In order that physical states have positive norm we must impose \( \text{Im}(b_n^*c_n) > 0 \), a possible choice being \( c_n = ib_n^{13} \).

The physical Hilbert space inner product is (4.9) and it is finite provided \( \{b_n, c_n\} \) are properly restricted, for example, by demanding that \( \sum_n (|b_n|^2 + |c_n|^2) < \infty \). Following (3.22), note however, that in order that (4.7) as a whole be in the Hilbert space of the self adjoint operator (2.8) we must have \( N(\chi) = \sum_n |\psi_{\chi n}(\chi)|^2 < \infty \). This condition will hold generally for finite values of \( \chi \) provided (4.3) is finite. However, from the asymptotic behavior of \( U_n \) and \( V_n \) we know that \( N(\chi) \) blows up like

\[13\]Note that using harmonic oscillator eigenstates for the \( \psi_{\chi n}(\chi) \) makes all states in (4.7) zero norm states in the same way that using (4.5) for the \( \psi_{\alpha n}(\alpha) \) renders all states (4.1) zero norm states.
\[ e^{x^2} \text{ as } |\chi| \to \infty \text{ throwing (4.7) out of the domain of (2.8) at } |\chi| = \infty, \text{ even though (4.9) remains finite. The limit } |\chi| \to \infty \text{ is easily attainable for any finite value of the scalar field } \phi \text{ as the scale factor } a \text{ blows up to infinity because } \chi = \pi a \phi. \text{ This apparent difficulty deserves further investigation, but we are not going to do so in this paper. We only mention that this problem can be avoided in the single tunneling wave function domain, because the single energy } E_0 \text{ can be always chosen as one of the harmonic oscillator eigenvalues with the corresponding square integrable } \psi_{\chi E_0}(\chi). \]

We see that a single (and relatively simple) physical system, namely, a conformal scalar field coupled to gravity, is described by two different and incompatible physical Hilbert spaces, corresponding to the two different possible time parametrizations. This implies that two highly different physical “realities” correspond to the same field theory coupled to gravity which in our opinion is an extreme manifestation of the problem of time in quantum gravity\(^{14}\).

In the model discussed above, time parametrization by the matter field \( \chi \) forces us to use the gravitational wave functions \( \psi^{(\alpha,\beta)}(\alpha a) \) in (4.6) (for \( a > a_2 \)) in constructing physical states (4.7) in the non trivial domain. This means that there is a continuum of distinct physical Hilbert spaces that are parametrized by the two real variables \( \alpha \) and \( \beta \) which are the domains for the non trivial self adjoint extensions of (2.8). Thus, specifying a physical state requires fixing \( \alpha \) and \( \beta \) first.

The most urging physical question that arises concerns the cosmological interpretation of \( \alpha \) and \( \beta \): is there really a continuum of distinct WDW operators or are these parameters fixed somehow by a yet unknown dynamical mechanism associated with quantum gravity\(^{15}\)? If there is such a continuum of WDW operators, which of them corresponds to the “real” Universe?

To partially answer these questions, recall that the wave function of the Universe is a unique solution of the WDW equation that must be singled out of all the other mathematically possible solutions whose general WKB form is (4.7). One then generally argues\(^{13}\) that the distinguished semiclassical solution which is the wave function

\(^{14}\) Using the terminology of Kuchař\(^\text{[12]}\), this is the “Multiple Choice Problem”.

\(^{15}\) As happens, for example, with the \( \theta \) angle in the Standard Model.
of the Universe will be picked up by matching it to a yet unknown solution of the
WDW equation corresponding to the exact theory of quantum gravity that governs
small geometries. In the case discussed here more is required, namely, that such a
matching condition will teach us something about $\alpha$ and $\beta$ as well. It might be that
the parameter $\beta$ is an artifact of our minisuperspace approach, because it defines the
boundary condition (3.15) at $a = 0$ where the RW minisuperspace approach as a
whole probably breaks down. Thus, it is plausible that if we knew the exact WDW
operator for small geometries the ambiguity associated with $\beta$ would be lifted either
by showing that $\beta$ is indeed a minisuperspace artifact, or by fixing its value if it has
anything to do with the exact Hamiltonian. Unfortunately, we cannot see how such
considerations apply as far as the parameter $\alpha$ is concerned. Indeed, $\alpha$ specifies the
boundary condition at $a \to \infty$ where the semiclassical approximation is perfectly
valid, and moreover, it is completely independent of $\beta$. It seems to us highly unlikely
that small geometry quantum gravity effects will be able to remove the ambiguity in
the WDW operator and the wave function of the Universe associated with $\alpha$.

As a matter of fact, $\alpha$ has the following interesting cosmological interpretation:
The original Hartle-Hawking wave function of the Universe \cite{19, 20, 11} $\Psi_{HH}(a > a_2) \sim
(|V(a)|)^{-1/4}\cos\left(\int_{a_2(E)}^{a} 4|V(y)|dy - \pi/4\right)$ is obtained from the semiclassical approx-
imation to the Euclidean path integral based on the “no boundary” proposal\cite{22}. It
is governed by one of the two Euclidean solutions to the classical equations of motion
having the larger action. It has been shown, however, in \cite{23} that the contribution to
the path integral from the other classical solution is relevant as well. It follows than,
that if one considers contributions to the path integral weighed by real coefficients,
one obtains a generalization of the Hartle-Hawking wave function given by (4.6) eval-
uated at $E = 0$. Thus, $\cos\phi_\alpha(0)$ weighs the contribution of the larger action saddle
point and $\sin\phi_\alpha(0)$ weighs the other one.

The “no boundary” proposal of Hartle and Hawking points at the special role
played by zero energy $E = 0$. It corresponds to regular Euclidean geometries, whereas
singular Lorentzian geometries occur for $E > 0$. Note further that $\beta$, whose inter-
pretation is problematic from cosmological point of view, disappears from (3.17) and (3.18) at $E = 0$. It is therefore interesting to study the consequences of including $E = 0$ in the discrete spectrum of (3.18). Using (3.13), (3.17) and (3.19) at $E = 0$ and demanding that (3.18) be satisfied at $E = 0$ as well, we obtain the following functional relation between $g^2$ and $\alpha$

$$\tan \left( \frac{C_\alpha}{g^2} \right) = -\frac{1}{4} \exp \left( -\frac{2}{3g^2} \right). \tag{4.10}$$

where $C_\alpha$ was defined following (3.13). Thus, for a given value of $\alpha$ (4.10) quantizes the cosmological constant $\Lambda = 3g^2$. Note further that (4.10) has a maximal positive solution $g^2_{\text{max}}$ which sets an upper bound for the cosmological constant. For realistic values of the cosmological constant $g^2 \ll 1$ Eq. (4.10) reduces to

$$\Lambda_n = \frac{3|C_\alpha|}{n\pi} , \quad n >> \frac{|C_\alpha|}{\pi} . \tag{4.11}$$

We close this section by making some comments regarding possible extension of our work. For simplicity, we have focused our discussion on RW cosmologies that are isotropic and homogeneous. Generalization of our work to more complicated cosmologies (presumably with positive cosmological constant) is clearly required. Moreover, implications of uniqueness of the tunneling wave function as the wave function of the Universe in case of time parametrization by matter fields to inflationary models should be clarified. Work on these points is in progress.

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A Appendix

Consider the self adjoint Hamiltonian \( H = \frac{1}{2m}P^2 + V(x) \); \( x \geq 0 \) and its domain \( \mathcal{D} \). We assume that \( V(x) \) is unbounded from below such that (1.9) holds. For simplicity we also assume that \( V(0) = 0 \) is a local extremum of \( V(x) \). We show in this appendix (within the framework of the WKB approximation) that if \( \mathcal{D} \) consists purely of right moving (or of left moving) waves, it is trivial, namely, a single ray. We also present indications that this is the case for generalized tunneling wave functions as well.

We first consider right moving waves, but the results are the same for left moving waves. Let \( x_>(E) \) be the largest turning point of a classical particle with energy \( E \) moving in a general potential \( V(x) \) satisfying (1.9). A right moving WKB solution to the right of \( x_>(E) \), is

\[
\Psi_E^{(WKB)}(x > x_>) = \frac{A_E}{[2m(E - V(x))]^{1/4}} \exp \left( i \int_{x_>(E)}^x \sqrt{2m(E - V(y))} dy \right),
\]

where \( A_E \) is a complex amplitude.

For energies above the maximum \( V_{\text{max}} \) of \( V(x) \) (that is \( E > \frac{1}{4g^2} \) in the case of (3.1)) there are no turning points and \( \Psi_{\text{WKB}} \) is the wave function for all \( x \geq 0 \) so that \( x_> = 0 \).

Consider the current

\[
J^{12}(x) = \frac{i}{2}(\Psi_2 \partial_x \Psi_1^* - \Psi_1^* \partial_x \Psi_2)(x).
\]

At \( x = 0 \) we have

\[
\left( J^{12}(0) \right)_{E > V_{\text{max}}} = \frac{1}{2} A_{E_1}^* A_{E_2} \left[ \left( \frac{E_1}{E_2} \right)^{1/4} + \left( \frac{E_2}{E_1} \right)^{1/4} \right]
\]

while for \( x \to \infty \) the current becomes

\[
J^{12}(x \to \infty) \to A_{E_1}^* A_{E_2} e^{-i\delta_{12}(\infty)}.
\]

Here \( \delta_{12}(x) = \int_{x_>(E_2)}^x \sqrt{2m(E_2 - V(y))} dy - \int_{x_>(E_1)}^x \sqrt{2m(E_1 - V(y))} dy \). From (A.3) and (A.4) we see that \( J^{12}(0) = J^{12}(\infty) \) if and only if \( E_1 = E_2 \), so \( \mathcal{D} \) contains at most only a single eigenstate in the energy range \( E > V_{\text{max}} \).

\[\text{Note further that } V''(0) > 0 \text{ is a necessary condition for } E \sim 0 \text{ to be in the spectrum.}\]
For energies below the lowest local minimum $V_{\text{min}}$ of $V(x)$ (that is, $E < 0$ in the case of (3.1)) there is only one turning point, $x_0(E)$, and the current at $x = 0$ is

\[
(J^{12}(x = 0))_{E < V_{\text{min}}} = \frac{1}{2} A^*_E A_E \left\{ \cosh(\xi_1 - \xi_2) \left[ \left( \frac{E_1}{E_2} \right)^{1/4} + \left( \frac{E_2}{E_1} \right)^{1/4} \right] \right.
\]

\[
- i \left( \frac{1}{4} e^{-(\xi_1 + \xi_2)} - e^{\xi_1 + \xi_2} \right) \left[ \left( \frac{E_2}{E_1} \right)^{1/4} - \left( \frac{E_1}{E_2} \right)^{1/4} \right] \right\},
\]

where $\xi_i = \int_{x_0}^{x(E)} \sqrt{2m(V(y) - E_i)} dy$. The norm squared of the current at $x = 0$ is

\[
|J^{12}(0)|^2_{E < V_{\text{min}}} = \frac{1}{4} |A^*_E A_E|^2 \left\{ \cosh^2(\xi_1 - \xi_2) \left( 2 + \sqrt{\frac{E_1}{E_2}} + \sqrt{\frac{E_2}{E_1}} \right) \right.
\]

\[
+ \left( \frac{1}{4} e^{-(\xi_1 + \xi_2)} - e^{\xi_1 + \xi_2} \right)^2 \left( \sqrt{\frac{E_1}{E_2}} + \sqrt{\frac{E_2}{E_1}} - 2 \right) \right\},
\]

while from (A.4) the norm squared at $x \to \infty$ is

\[
|J^{12}(x \to \infty)|^2 = |A^*_E A_E|^2.
\]

The last two expressions are equal if and only if $E_1 = E_2$ and thus also in this energy range $D$ contains at most a single eigenstate.

For energies in the range $V_{\text{min}} < E < V_{\text{max}}$ there are more turning points and $J^{12}(0)$ is sensitive to the details of the potential, but one can show that the domain $D$ is trivial as well. For concreteness let us consider the potential (3.1). In the energy range $0 < E < \frac{1}{4}g^2$ there are two (positive) turning points, $0 < x_- < x_+$. Using the WKB matching conditions, the wave function to the left of $x_-(E)$ which corresponds to (A.1) is

\[
\Psi_E^{(WKB)}(x < x_-) = \frac{-A_E e^{i\pi/4}}{[2m(E - V(x))]^{1/4}} \left\{ \frac{e^{-\Delta(E)}}{2} \sin[\phi_E(x)] + 2ie^{\Delta(E)} \cos[\phi_E(x)] \right\},
\]

where $\phi_E(x) = \int_{x_-}^{x} \sqrt{2m(E - V(y))} dy - \frac{\pi}{4}$ and $\Delta(E)$ is given by (3.19). The current at $x = 0$ becomes

\[
J^{12}(0) = \frac{1}{2} A^*_E A_E \left\{ \left[ (c_{12} + c_{12}^{-1}) \cos \phi_1 \cos \phi_2 \right.ight.
\]

\[
+ (d_{12} + d_{12}^{-1}) \sin \phi_1 \sin \phi_2 \left. \right\} - i \left[ (a_{12} + a_{12}^{-1}) \cos \phi_1 \sin \phi_2 \right.
\]

\[
- (b_{12} + b_{12}^{-1}) \sin \phi_1 \cos \phi_2 \left. \right\},
\]

\[27\]
where

\[
a_{12} = \frac{1}{4} \left( \frac{E_1}{E_2} \right)^{1/4} e^{-(\Delta(E_1)+\Delta(E_2))}, \quad b_{12} = \frac{1}{4} \left( \frac{E_2}{E_1} \right)^{1/4} e^{-(\Delta(E_1)+\Delta(E_2))}\n\]

\[
c_{12} = \left( \frac{E_1}{E_2} \right)^{1/4} e^{-(\Delta(E_1)−\Delta(E_2))}, \quad d_{12} = \left( \frac{E_2}{E_1} \right)^{1/4} e^{-(\Delta(E_1)−\Delta(E_2))},
\]

and

\[
\phi_i = \phi_{E_i}(0) = \frac{\sqrt{2m x_2(E_i)}}{3g} \left[ \mathcal{E} \left( \frac{x_1(E_i)}{x_2(E_i)} \right) - \sqrt{1 - 4E_i g^2 K \left( \frac{x_1(E_i)}{x_2(E_i)} \right)^2} \right] - \frac{\pi}{4}. \quad (A.11)
\]

The norm squared of (A.9) can be written in the form

\[
|J^{12}(0)|^2 = \frac{1}{4} |A_{E_1} A_{E_2}|^2 \left\{ (c_{12} + c_{12}^{-1})^2 \cos^2 \phi_1 + (d_{12} + d_{12}^{-1})^2 \sin^2 \phi_1 \right. \]

\[+ \left. \left[ (a_{12} + a_{12}^{-1}) \cos \phi_1 \sin \phi_2 - (b_{12} + b_{12}^{-1}) \sin \phi_1 \cos \phi_2 \right]^2 \right. \]

\[\left. - \left[ (c_{12} + c_{12}^{-1}) \cos \phi_1 \sin \phi_2 - (d_{12} + d_{12}^{-1}) \sin \phi_1 \cos \phi_2 \right]^2 \right\}. \quad (A.12)
\]

For fixed \(E_1\) one may consider the right hand side of (A.12) as a function of \(E_2\). Using (A.11),(A.11) and (3.19) it can be shown that this function has a global minimum at \(E_2 = E_1\) where trivially \(J^{11}(0) = J^{11}(\infty)\). Thus, for any other \(E_2 \neq E_1\) (in this energy range) we have \(|J^{12}(0)| > |J^{12}(\infty)|\) and (3.6) does not hold. Therefore \(D\) contains a single eigenstate in this \(E\) range as well.

So far we saw that \(D\) contains at most a single eigenstate in each of the energy ranges \(E < V_{\text{min}}, V_{\text{min}} < E < V_{\text{max}}\) and \(E > V_{\text{max}}\). Considering now self adjointness of the Schrödinger operator in this finite dimensional domain \(D\) we easily see that \(D\) is actually only one dimensional (because otherwise \(|J^{12}(0)| > |J^{12}(\infty)|\) for any pair of different such states) and the spectrum of \(H\) shrinks to a single point \(E = E_0\).

For generalized tunneling wave functions which are not purely right (or left) moving waves, the explicit form of the (non-zero) \(J^{12}(0)\) is more complicated and we currently do not have a complete proof that \(D\) is one dimensional, but we present below indications that it is finite dimensional at most. The WKB wave function to the right of the largest turning point is

\[
\Psi_E^{(WKB)}(x > x_{\text{r}}) = \frac{1}{(E - V(x))^{1/4}} \left[ A_{E} \exp \left( i \int_{x_{\text{r}}}^{x} \sqrt{2m(E - V(y))} dy \right) \right]
\]

28
where $A_E$ and $B_E$ are complex amplitudes. For self adjoint Hamiltonians with potentials satisfying (1.9) that are defined over an infinite dimensional domain $D$ the spectrum is necessarily unbounded from below and from above. In this case one can choose two eigenstates in $D$ with energies $E_1$ and $E_2$ above $V_{\text{max}}$, such that $E_2/E_1 \to \infty$. To leading order in $(E_1/E_2)^{1/2} \ll 1$ the current at $x = 0$ is

$$J^{12}(0) \sim \frac{1}{2} \left( \frac{E_2}{E_1} \right)^{1/4} \left( A^*_{E_1} A_{E_2} - B^*_{E_1} B_{E_2} + B^*_{E_1} A_{E_2} - A^*_{E_1} B_{E_2} \right).$$  (A.14)

On the other hand, the current at infinity is

$$J^{12}(x \to \infty) \to A^*_{E_1} A_{E_2} e^{-i\delta_{12}} - B^*_{E_1} B_{E_2} e^{i\delta_{12}}.$$  (A.15)

A generalized tunneling wave function is a wave function for which $|A_E| > |B_E|$. For such wave functions the norm of (A.14) diverges as $E_2/E_1 \to \infty$, while the norm of (A.13) is finite. Thus, $J^{12}(0) \neq J^{12}(\infty)$ and therefore, contrary to our initial assumption, the spectrum has to be bounded from above. Similarly, using (A.6) for negative energies we find that $J^{12}(0)$ diverges when $|E_2|/|E_1| \to \infty$, and the spectrum must be bounded from below as well. There must be a finite minimum gap between energy levels in the band $0 < E < \frac{1}{2g^2}$ and thus the number of eigenstates is finite at most. Because this argument involves the limit $E_2 \to \infty$ it is insensitive to the details of $V(x)$ near $x = 0$ as long as $V(x)$ and $V'(x)$ are regular at the origin.

$J^{12}(x = 0)$ can be equal to $J^{12}(x \to \infty)$ for $E_2/E_1 >> 1$ only if they are both zero. Only in this case $J^{12}(x = 0)$ will not diverge as $E_2/E_1 \to \infty$, and we can have a non-trivial (infinite dimensional) domain for the self-adjoint Hamiltonian. This was studied in section 3.
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