Chaos and Semiclassical Limit in Quantum Cosmology

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Abstract

In this paper we present a Friedmann-Robertson-Walker cosmological model conformally coupled to a massive scalar field where the WKB approximation fails to reproduce the exact solution to the Wheeler-DeWitt equation for large Universes. The breakdown of the WKB approximation follows the same pattern than in semiclassical physics of chaotic systems, and it is associated to the development of small scale structure in the wave function. This

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result puts in doubt the “WKB interpretation” of Quantum Cosmology.
I. INTRODUCTION

Quantum Cosmology \[1\] tries to provide a complete description of the universe. Since the present universe obeys classical laws with great precision, an acceptable Quantum Cosmology must predict a “quantum to classical” transition at a certain time in the cosmic evolution. In the same manner, it must provide an interpretation of the initial conditions of the classical evolution, in terms of quantum processes. For these reasons, it is clear that the problem of the correspondence between classical and quantum behavior is a central point in the development of quantum cosmology.

To explain our observations it is enough to interpret the wave function of the universe in the semiclassical limit \[2\]. Moreover, it has been argued that it is sufficient to have a Wentzel-Kramers-Brillouin (WKB) state or a Gaussian state to have a valid semiclassical description \[3\]. This is the basis of the so-called “WKB interpretation of Quantum Cosmology”. According to this interpretation, we can understand the semiclassical limit as the limit $m_p \rightarrow \infty$, where $m_p$ stands for the Plank mass. In this limit the wave function of the universe, may be understood as a superposition of solutions of the WKB type \[4\],

$$
\Psi = \sum \alpha C_\alpha \exp \left[ \frac{i}{\hbar} S_\alpha \right]
$$

where the $S_\alpha$ are solutions to the classical Hamilton Jacobi equation and the $|C_\alpha|^2$ may be interpreted as the relative probability the $\alpha$ classical solution. However, we want to obtain the semiclassical limit when the universe has expanded beyond a certain size, and not in the limit $m_p \rightarrow \infty$. The $m_p \rightarrow \infty$ limit of the wave function of the Universe would provide nevertheless information on the large size behavior, if the limits $m_p \rightarrow \infty$ and $a \rightarrow \infty$ commuted, where $a$ stands for the radius of the universe in a Robertson-Walker model. Although more recent papers have suggested the necessity of including decoherence to the WKB limit, in order to obtain a truly semiclassical state \[4\], it is commonly assumed in the literature on quantum cosmology that the wave function of the universe adopts a WKB form at some point in the cosmic evolution, and retains it for ever after.
This problem is similar to the problem of the commutativity of the limits \( \hbar \to 0 \) and \( t \to \infty \) in ordinary quantum mechanics. The semiclassical wave function has been studied in great detail, and it has been shown that for irregular systems (chaotic systems) there exists a breakdown of the validity of the WKB approximation [6,7]. The existence of chaotic cosmologies [8] suggests that a similar breakdown in the WKB approximation might occur in cosmological models. This would put in doubt the WKB interpretation of quantum cosmology.

However, the problem of quantum cosmology cannot be referred directly to the quantum mechanical problem, because the Wheeler-DeWitt equation, the equation that governs quantum cosmology, is of second order. Therefore, we need to analyze the problem from first principles; it is convenient to begin such analysis with a simple, exactly solvable model.

In this paper, we present such a model, namely a spatially flat Friedmann-Robertson-Walker (FRW) model coupled to a scalar field. Choosing a suitable coupling of the field to the radius \( a \) of the universe, we solve the Wheeler-DeWitt equation exactly. For the same model we calculate the semiclassical wave function, and we compare the evolution of this wave function with the exact one, checking the validity of the WKB approximation.

The results obtained in this paper confirm the suspicion that the WKB approximation breaks down in quantum cosmology for large universes. This puts in doubt the WKB interpretation in its original formulation. The WKB approximation may still be valid, however, in more realistic models, for example, those including decoherence.

II. THE MODEL

Our cosmological model assumes a FRW spatially flat geometry, conformally coupled to a real massive scalar field \( \Phi \). We shall suppose a \( \Phi(r, \eta) = \exp(i k r) \phi(\eta)/a(\eta) \), with \( k \ll 1 \). This is a dynamical system with two degrees of freedom, \( a \) and \( \phi \), and Hamiltonian [8]

\[
H = \frac{1}{2} \left\{ \frac{-P_a^2}{m_p^2} + \pi_\phi^2 + [k^2 + m^2 V(a)]\phi^2 \right\} = 0
\] (2)

Where \( \pi_\phi \) and \( P_a \) are the momenta conjugated to \( \phi \) and \( a \) respectively.
For the numerical calculation we choose the potential

\[ V(a) = \sum_{n=1}^{\infty} (2n - 1) \Theta(|a| - \delta a)n \delta a^2 \]  

(3)

where \( \Theta(x) \) is the Heaviside step function and \( \delta a \) is the step length (Fig. 1).

Introducing dimensionless variables \( P_a/m_p k^2 \to P_a, a m_p/k \to a, \pi_\phi/k^2 \to \pi_\phi, \phi/k \to \phi, m/m_p \to m \), the adimensional Hamiltonian reads

\[ H = \frac{1}{2} \{-P_a^2 + \pi_\phi^2 + [1 + m^2 \sum_{n=1}^{\infty} (2n - 1) \Theta(|a| - \delta an) \delta a^2] \phi^2 \} = 0 \]  

(4)

We can reduce the system's freedoms by one, using the Hamiltonian constraint. Hamilton's equations for the reduced system in the range \( n \delta a < a \leq (n+1) \delta a \), are

\[ \frac{d\phi}{da} = \frac{\delta h}{\delta \pi} = \frac{\pi}{\sqrt{\pi^2 + \omega_n^2 \phi^2}} = \frac{\pi}{E_n} \]  

(5)

\[ \frac{d\pi}{da} = -\frac{\delta h}{\delta \phi} = \frac{-\omega_n^2 \phi}{\sqrt{\pi^2 + \omega_n^2 \phi^2}} = -\frac{\omega_n^2 \phi}{E_n} \]  

(6)

Where now \( a \) plays the role of time, \( h = -P_a = E_n = \sqrt{\pi^2 + \omega_n^2 \phi^2} \) and

\[ \omega_n(a) = [1 + m^2 n^2 \delta a^2]^{1/2} \]  

(7)

is the frequency in each step. These equations of motion correspond to an harmonic oscillator of frequency \( \frac{\omega_n}{E_n} \), so the solution for the reduced system is

\[ \phi^{(n)}(\delta a) = \phi^{n+1} = \phi^n \cos\left(\frac{\omega_n}{E_n} \delta a\right) + \frac{\pi_n}{\omega_n} \sin\left(\frac{\omega_n}{E_n} \delta a\right) \]  

(8)

\[ \pi^{(n)}(\delta a) = \pi^{n+1} = -\omega_n \phi^n \sin\left(\frac{\omega_n}{E_n} \delta a\right) + \pi^n \cos\left(\frac{\omega_n}{E_n} \delta a\right) \]  

(9)

These equations define a stroboscopic map of period \( \delta a \), where \( \phi^n \) and \( \pi^n \) are the values of the field and its conjugated momentum in the border of the \( n \)th step.

As we cross the threshold from one step to the next, the energy changes from \( E_n \) to \( E_{n+1} \). This non-conservation of the energy is a signal of the non-integrability of this model.
A. Semiclassical Wave Function

Having found the solution to the classical problem we proceed to construct the semiclassical wave function as discussed by Berry [6]. The idea is to associate wave functions $\Psi(\phi)$ to N-dimensional Lagrangian surfaces $\Sigma$, in the phase space $(\phi, \pi_\phi)$ (in our case, N=1). The association between $\Sigma$ and $\Psi$ is purely geometric, the dynamics of the problem will be introduced later, when we evolve the surface. We take the initial surface $\Sigma_o$ as the invariant curve of the classical Hamiltonian for a massless field ($m=0$).

\[
h^2 = \pi_\phi^2 + \phi^2 = E_o^2 \tag{10}
\]

Where $E_o = 2\omega_o(k+1)$, $\omega_o = 1$, and $k$ is a natural number, as in Sommerfeld quantization rules.

Our task is to associate $\Sigma$ to a wave function

\[
\Psi(\phi) = A(\phi) \exp(iS(\phi)) \tag{11}
\]

Where $A(\phi) = K\left| \frac{\delta^2 S}{\delta \phi \delta I} \right| = K\left| \frac{d\varphi}{d\phi^o} \right| = K\left| \frac{\omega_o}{\pi_o} \right| \tag{12}$

with $K$ a constant of proportionality, and $S$ is a solution of the classical Hamilton Jacobi equation, parametrized by $I$.

If we now generalize this to a curve $\Sigma_n$, obtained by evolving $\Sigma_o$ n times through the classical map of equations (8) and (9), the probability density associated to $\Sigma_n$ is given by

\[
A_n^2 = \left| \frac{d\varphi}{d\phi_n} \right| = \left| \frac{d\varphi^o}{d\phi^o} \right| = A_o^2 \left| \frac{d\phi^o}{d\phi_n} \right| \tag{13}
\]

To obtain the phase of the associated wave function we proceed as follows. The phase difference between two points separated $\delta \phi$ on the surface $\Sigma$ is

\[
\Delta S_o = S_o(\phi^o, I) - S_o(0, I) = \int_0^{\phi^o} \pi_o d\phi^o = \int_0^{\phi} 2I \cos^2(\varphi) d\varphi = I\varphi + \frac{I}{2\sin(2\varphi)} \tag{14}
\]
And the phase difference between two points on the curve \( \Sigma_n \) (fig.2), reads

\[
\Delta S_n = \Delta S_{n-1} + \frac{1}{2}(\pi \phi^n - \pi \phi^{n-1} - \phi^n - \phi^{n-1} - E_n \delta a)
\]

(15)

Where we neglected a global phase \( \sigma_n(\phi^n(0), I) \).

Since the function \( \pi^n(\phi) \) is multivalued, the wave function corresponding to the curve \( \Sigma_n \) is given by the superposition principle as

\[
\Psi^n(\phi) = \sum_{\alpha} A_{\alpha}^n(\phi) \exp[i\hat{S}_{\alpha}(\phi, I) + \frac{\pi}{2}\mu]
\]

(16)

where \( \alpha \) labels the different branches of \( \Sigma_n \) for a given value of \( \phi \), and \( \mu \) is the Maslov index associated to each fold of the curve \( \Sigma_n \).

**B. Solution to the Wheeler-DeWitt Equation**

Following the canonical quantization procedure, we obtain the Wheeler-DeWitt equation for this model:

\[
\frac{1}{2}\left[ \frac{\delta^2}{\delta a^2} - \frac{\delta^2}{\delta \phi^2} + \omega_n^2(a)\phi^2 \right] \Psi(a, \phi) = 0
\]

(17)

where \( \omega_n(a) \) is defined in eq.(8) and we have chosen the factor ordering so that the term in second derivatives becomes the Laplacian operator in the minisuperspace metric. Within the range \( n\delta a \leq a < (n+1)\delta a \), we may expand

\[
\Psi_n(a, \phi) = \sum_{j}^\infty [A_n^j F_n^j+(a, \phi) + B_n^j F_n^j-(a, \phi)]
\]

(18)

where

\[
F_n^j(\phi) = \frac{1}{\sqrt{2} \sqrt[4]{E_n^j}} \exp[\mp i \sqrt{E_n^j a}] \Phi_n^j(\phi)
\]

(19)

and

\[
\Phi_n^j(\phi) = \left( \frac{\omega_n}{\pi} \right)^{1/4} \frac{1}{(2j!)^{1/2}} \exp[-\frac{1}{2} \omega_n \phi^2] h^j(\sqrt{\omega_n} \phi)
\]

(20)

where \( h_j(x) \) is the Hermite polynomial of grade \( j \) and \( E_n^j = \omega_n(2j + 1) \).
Asking for continuity in the wave function and its normal derivative at the border of each step, we obtain the recurrence formulae for the coefficients of the expansion

\[ A_{n+1}^i = \sum_{j}^{\infty} [A_n^j(F_{n+1}^{i^+}, F_{n}^{j^+}) + B_n^j(F_{n+1}^{i^+}, F_{n}^{j^-})] \] (21)

\[ B_{n+1}^i = \sum_{j}^{\infty} [A_n^j(F_{n+1}^{i^-}, F_{n}^{j^+}) + B_n^j(F_{n+1}^{i^-}, F_{n}^{j^-})] \] (22)

Where \((g, f)\) is the Klein Gordon inner product

\[ (g, f) = i \int d\phi (g^* \frac{\delta f}{\delta a} - f \frac{\delta g^*}{\delta a}) \] (23)

From the equations (18) to (23) we finally obtain \(\Psi_n(a, \phi)\) at the border of each step, from which we calculate \(|\Psi_n(a^*, \phi)|^2\}. This squared amplitude will be compared to that of the Semiclassical wave function. Also, we obtain the Klein Gordon charge, defined by the scalar product of eq.(23) as \(Q_n = (\Psi_n(a, \phi), \Psi_n(a, \phi))\). This charge is conserved by the Wheeler-DeWitt equation. We shall present the details of this recurrence relations in Appendix A.

### III. RESULTS

Figures 3b and 5b show unfolding of the curve \(\Sigma\) evolved from an initial curve \(\Sigma_0\) through the classical map of eqs.(8) and (9). The most outstanding feature is the development of spiral structures or “whorls”, as Berry calls them [6]. These are associated with invariant curves around a stable fixed point of \(h\). They can arise, for example, in the twist map [14], provided the angular frequency depends on the radius. In this case, points at different radii rotate around the central fixed point at different rates. Therefore radii map to spirals, and parts of \(\Sigma\) traveling close to stable fixed points will wrap around them, as it can be seen in figures 3b and 5b. For these two figures (3 and 5) we chose two different values of \(\delta a\), \(\delta a = 0.5\) and \(\delta a = 0.25\) respectively. By the 10th step the ”spiral galaxy” structure is clearly visible in the 3b curves. For the curves of figure 3b, the spiral galaxy structure is visible
already at the 20th step (it must be noted that $n = 10$ and $n = 20$ correspond to the same “time” of evolution for the different figures), in spite of having a smoother potential.

In figures 3a and 5a we can appreciate the semiclassical wave functions associated to the phase curves in figures 3b and 5b respectively. The most striking features are the caustic spikes, which proliferate as $n$ increases and the classical curves curl over.

The graphs of $|\Psi|^2$, obtained from the exact solutions of the Wheeler-DeWitt equation, are shown in figures 4b and 6b for two different values of $\delta a$, $\delta a = 0.5$ and $\delta a = 0.25$ respectively. To study the corresponding quantum map (i.e. eq. 18) we must choose as initial state $\Psi_0$ a wave function associated to $\Sigma_0$. Because $\Sigma_0$ is an invariant curve of $h_0$, $\Psi_0$ must be an eigenstate of this operator. For the curves mapped on figures 4b and 6b, $\Psi_0$ was chosen to be the 5th eigenstate of $h_0$. The graph of $|\Psi|^2$ for $n = 0$ clearly shows the association with the initial curve $\Sigma_0$, with maxima at the caustics of the projection of $\Sigma$, and, between these, near harmonic oscillations. These oscillations correspond to the interference of two waves, associated with the intersection of $\pi_i(\phi)$ with the fiber $\phi = \text{constant}$, which make up the WKB function of figs. 3a and 5a.

By the 10th iteration (20th for $\delta a = 0.25$) the WKB $|\Psi|^2$ (figs. 3a (resp. 3a)) has developed a complexity which cannot be observed in the real $|\Psi|^2$. The caustics are evidently related to features of the wave function until $n = 10$ (resp. $n = 20$) but thereafter there is no obvious association. This is related to the fact that for large $n$ the neighboring caustics in fig.3a (resp. fig.5a) are closer than the de Broglie wavelength, so they cannot be associated with features of $\Psi$. This suggests, in the spirit of the smoothing procedure, that a better match between classical and quantal calculations will be obtained if we smooth, in some sense, the graph of $|\Psi|^2$. Decoherence, or some other process that can eliminate details of the WKB function, could provide a suitable smoothing mechanism.

In our numerical calculation of the exact wave function, we have computed only the first 100 terms of the defining series eq. (18). As a check that this truncation does not impair the accuracy of our results, we show in figs. 4a and 6a a logarithmic plot of these coefficients. It is clearly seen from these plots that the coefficients decay exponentially, thus ensuring that
the tail of the series does not influence the value of the wave function within the accuracy of our calculations. Observe that the decay of the expansion coefficients for \( \delta a = 0.25 \) (fig.6a) is markedly faster than for \( \delta a = 0.5 \) (fig.6a), as we should expect for a smoother evolution. As another check of the numerical accuracy, we computed the Klein Gordon charge for each step, verifying that it was conserved.

**IV. DISCUSSION**

In this paper we have presented a simple cosmological model where the WKB approximation fails to reproduce the exact solution to the Wheeler-DeWitt equation for large Universes. The breakdown of the WKB approximation follows the same pattern than in semiclassical physics of chaotic systems, and it is associated to the development of small scale structure in the wave function. This result puts in doubt the so-called “WKB interpretation of Quantum Cosmology”, at least in its original formulation \[3\]. More complex models may provide a smoothing mechanism for the wave function, thus restoring the WKB approximation.

In this model, the breakdown of the WKB approximation follows from the joint action of two effects, namely, the twist caused by the dynamics within each step, and the “particle creation” effect, that produces the excitation of higher eigenstates at each threshold. Since each of these effects are present in the continuum limit, \( \delta a \to 0 \), we may conclude that the WKB approximation will not be restored there. This is put into evidence by the fact that halving \( \delta a \) leads to a stronger, rather than weaker, failure of the WKB approximation.

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APPENDIX A: RECURRENCE FORMULAE FOR THE EXACT WAVE FUNCTION

The scalar products in equations \( (22) \) and \( (23) \) may be computed from the recurrence relations

\[
(F_{n+1}^i, F_n^j) = \left[ \sqrt{E_{n+1}^i} + \sqrt{E_n^j} \right] \frac{\exp[i(\sqrt{E_{n+1}^i} - \sqrt{E_n^j})a^*]}{2(E_{n+1}^i E_n^j)^{1/4}} (n + 1; i|n; j) \tag{A1}
\]

\[
(F_{n+1}^{i+}, F_n^j) = \left[ \sqrt{E_{n+1}^i} - \sqrt{E_n^j} \right] \frac{\exp[i(\sqrt{E_{n+1}^i} + \sqrt{E_n^j})a^*]}{2(E_{n+1}^i E_n^j)^{1/4}} (n + 1; i|n; j) \tag{A2}
\]

\[
(F_{n+1}^i, F_n^{j-}) = \left[ -\sqrt{E_{n+1}^i} + \sqrt{E_n^j} \right] \frac{\exp[i(-\sqrt{E_{n+1}^i} - \sqrt{E_n^j})a^*]}{2(E_{n+1}^i E_n^j)^{1/4}} (n + 1; i|n; j) \tag{A3}
\]

\[
(F_{n+1}^i, F_n^{j-}) = \left[ -\sqrt{E_{n+1}^i} - \sqrt{E_n^j} \right] \frac{\exp[i(-\sqrt{E_{n+1}^i} + \sqrt{E_n^j})a^*]}{2(E_{n+1}^i E_n^j)^{1/4}} (n + 1; i|n; j) \tag{A4}
\]

In these equations,

\[
\langle n + 1; i|n; j \rangle = \int dx \Phi_{n+1}^i(x) \Phi_n^j(x) \tag{A5}
\]

These brackets can be written in recursive form

\[
\langle n + 1; j|n; i \rangle = \frac{\beta_n}{\alpha_n} \sqrt{\frac{j - 1}{j}} \langle n + 1; j - 2|n; i \rangle + \frac{1}{\alpha_n} \sqrt{i/j} \langle n + 1; j - 1|n; i - 1 \rangle \tag{A6}
\]

for \( i \leq j \), and

\[
\langle n + 1; j|n; i \rangle = -\frac{\beta_n}{\alpha_n} \sqrt{\frac{i - 1}{i}} \langle n + 1; j|n; i - 2 \rangle + \frac{1}{\alpha_n} \sqrt{j/i} \langle n + 1; j - 1|n; i - 1 \rangle \tag{A7}
\]

if \( j \leq i \), where \[15\]

\[
\langle n + 1; 0|n; 0 \rangle = \sqrt{\frac{1}{\alpha_n}} \tag{A8}
\]

and

\[
\alpha_n = \frac{1}{2} \left[ \sqrt{\frac{\omega_{n+1}}{\omega_n}} + \sqrt{\frac{\omega_n}{\omega_{n+1}}} \right] \tag{A9}
\]

\[
\beta_n = \frac{1}{2} \left[ -\sqrt{\frac{\omega_{n+1}}{\omega_n}} + \sqrt{\frac{\omega_n}{\omega_{n+1}}} \right] \tag{A10}
\]

\( \omega_n \) is the step frequency given in eq. \[7\]
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FIGURES

FIG. 1. Comparison of the potential $V(a) = a^2$ with the potential of the equation (3).

FIG. 2. The difference of phase between two points on the curve $\Sigma_n$ may be computed as the difference of phase on the curve $\Sigma_{n-1}$ plus the phase gain from evolution in $\delta a$.

FIG. 3. (a) Semiclassical Wave Function associated with the evolution of the curve $\Sigma$ for a value of $\delta a = 0.5$. (b) Evolution of the curve $\Sigma$ through the classical map, defined in equations (8) and (9), for a value of $\delta a = 0.5$.

FIG. 4. (a) Weight of the coefficients of the defining series of equation (18) for a value of $\delta a = 0.5$. (b) Evolution of the exact Wave Function of the Universe through the quantum map, defined in equation (18), for a value of $\delta a = 0.5$.

FIG. 5. (a) Semiclassical Wave Function associated with the evolution of the curve $\Sigma$ for a value of $\delta a = 0.25$. (b) Evolution of the curve $\Sigma$ through the classical map, defined in equations (8) and (9), for a value of $\delta a = 0.25$.

FIG. 6. (a) Weight of the coefficients of the defining series of equation (18) for a value of $\delta a = 0.25$. (b) Evolution of the exact Wave Function of the Universe through the quantum map, defined in equation (18), for a value of $\delta a = 0.25$. 
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$V(a) = a^2$
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\[ \sigma_n(0) \]

\[ \Delta S_{n-1} \]

\[ \Delta S_n \]

\[ \Sigma_{n-1} \]

\[ \Sigma_n \]

\[ \pi \]

\[ \phi \]

\[ a \]
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(a)

(b)
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\begin{align*}
|A|^2 + |B|^2 & \quad (n = 0) \\
|A|^2 + |B|^2 & \quad (n = 10) \\
|A|^2 + |B|^2 & \quad (n = 20) \\
|A|^2 + |B|^2 & \quad (n = 30)
\end{align*}