Wave packets and initial conditions in quantum cosmology

S. S. Gousheh and H. R. Sepangi*
Department of Physics, Shahid Beheshti University, Evin, Tehran 19839, Iran

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Abstract

We discuss the construction of wave packets resulting from the solutions of a class of Wheeler-DeWitt equations in Robertson-Walker type cosmologies. We present an ansatz for the initial conditions which leads to a unique determination of the expansion coefficients in the construction of the wave packets with probability distributions which, in an interesting contrast to some of the earlier works, agree well with all possible classical paths. The possible relationship between these initial conditions and signature transition in the context of classical cosmology is also discussed.

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1 Introduction

The question of the construction and interpretation of wave packets in quantum cosmology has been attracting much attention in recent years. Numerous studies have been done to obtain a quantum theory for gravity and to understand its connection with classical physics. This interest is due to our desire for obtaining the basic dynamical laws for predicting the large scale structure of the universe and the determination of the initial conditions from which the universe has evolved. The latter is of particular importance since if we accept that the fundamental laws of physics are quantum mechanical in nature, then the question of initial conditions is embodied in finding the initial condition for the quantum cosmological state of the universe, see for example [1]. The search for the fundamental dynamical laws has been underway since Newtonian times but that for the initial conditions is relatively recent and great efforts have been made in this direction. This is, of course, not surprising as the underlying theories for

*email: hr-sepangi@cc.sbu.ac.ir
describing the fundamental laws of physics are local quantum field theories above the Plank length. However, theories explaining the initial quantum state of the universe are non-local. They imply regularities in space that have emerged on large cosmological scales. It is only in recent years that the progress in observational cosmology on large enough scales of both space and time may present us with the opportunity to look at the viability of the predictions of a theory of the initial state of the universe.

The problem of the relation between quantum cosmology and classical physics is an important one that exists even in simple models [2]. Most authors consider semi-classical approximations to the Wheeler-DeWitt (WD) equation and refer to regions in configuration space where these solutions are oscillatory or exponentially decaying as representing classically allowed or forbidden regions, respectively. These regions are mainly determined by the initial conditions for the wave function. Two popular proposals for the initial conditions are the no boundary proposal [3] and the spontaneous nucleation from nothing [4]. These proposals have been attractive to many authors because they lead to some classes of classical solutions represented by certain trajectories which possess important features such as predicting an inflationary phase.

In quantum cosmology, in analogy with ordinary quantum mechanics, one is generally concerned with the construction of wave functions by the superposition of the ‘energy eigenstates’ which would peak around the classical trajectories in configuration space. However, contrary to ordinary quantum mechanics, a parameter describing time is absent in quantum cosmology so that the initial conditions would have to be expressed in terms of an intrinsic time parameter, which in the case of the WD equation could be taken as the local scale factor for the three geometry [5]. Also, since the sign of the kinetic term for the scale factor is negative, a formulation of the Cauchy problem for the WD equation is possible. The existence of such a sign is one of the exclusive features of gravity with many other interesting implications.

The construction of wave packets resulting from the solutions of the WD equation has been a feature common to most of the recent research work in quantum cosmology [6, 7, 8]. In particular, in reference [6] the construction of wave packets in a Friedmann universe is presented in detail and appropriate boundary conditions are motivated. Generally speaking one of the aims of these investigations has been to find wave packets whose probability distributions coincide with the classical paths obtained in classical cosmology. In these works, the authors usually consider model theories in which a self interacting scalar field is coupled to gravity in a Robertson-Walker type universe. The resulting WD equation is often in the form of an isotropic oscillator-ghost-oscillator and is separable in the configuration space variables. The general solution can thus be written as a sum over the product of simple harmonic oscillator wave functions with different frequencies. As usual, the coefficients in the sum are chosen according to the initial conditions, which are usually specified by giving the wave function at $R = 0$, where $R$ is the scale factor. The choice of the initial conditions, or equivalently the coefficients in the sum, varies considerably amongst various authors. In [6, 7], the wave packets are constructed by summing over the first few terms with the coefficients being chosen arbitrarily to be equal. However, in [3] the initial state is chosen to be a Gaussian with the appropriate symmetry and the undetermined coefficients being set to zero. The resulting wave packets, in general, lack one or more of the following desired properties. Firstly, one expects the wave packet describing a physical system to possess a certain degree of smoothness. Secondly, there should be a good classical-quantum correspondence, which means that not only the
wave packet should be centered around the classical path, but also the crest of the probability distribution should coincide as closely as possible with the classical trajectory. Also, to each distinct classical path there should correspond a unique wave packet.

The purpose of this paper is to address and clarify some of these issues. We first argue that specifying the wave function at \( R = 0 \) does not furnish a complete set of initial conditions. We then suggest an ansatz for the expansion coefficients, or equivalently for the initial conditions, which produces wave packets with the desired properties mentioned above. The organization of the paper is as follows: In section two we give a short review of some of the models that lead to the class of WD equations considered here. Section three deals with the construction of the wave packets and in section four we discuss the salient features of this work and conclusions are drawn.

## 2 Robertson-Walker cosmology with coupled scalar field

In Robertson-Walker cosmology, one often considers the coupling of a scalar field to gravity. The resulting field equations include a ‘zero energy constraint’. The WD equation in quantum cosmology is the result of the quantization consistent with this constraint. In some simple minisuperspace models the solutions to the WD equation describe a system of oscillators with unequal or equal frequencies. It would therefore be appropriate at this point to give a brief review of some of the minisuperspace models leading to the class of WD equations whose solutions are to be discussed here.

Consider Einstein’s field equation coupled to a scalar field

\[
\begin{align*}
R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R &= \kappa T_{\mu\nu}(\phi), \\
\Delta^2 \phi - \frac{\partial U}{\partial \phi} &= 0,
\end{align*}
\]

where \( T_{\mu\nu} \) is the energy-momentum tensor coupling the scalar field \( \phi \) to gravity and \( U \) is a scalar potential for the scalar field \( \phi \). Hereafter, we shall work in a system of units in which \( \kappa = 1 \). We parameterize the metric as

\[
g = -dt^2 + R^2(t) \frac{\sum dr^i dr^i}{(1 + kr^2/4)^2},
\]

where \( R(t) \) is the usual scale factor and \( k = +1, 0, -1 \) corresponds to a closed, flat or open universe respectively. The field equations resulting from (1) and (2) with the metric given by (3) can be written as

\[
\begin{align*}
3 \left[ \left( \frac{\dot{R}}{R} \right)^2 + \frac{k}{R^2} \right] &= \frac{\dot{\phi}^2}{2} + U(\phi), \\
2 \left( \frac{\ddot{R}}{R} + \left( \frac{\dot{R}}{R} \right)^2 + \frac{k}{R^2} \right) &= -\frac{\dot{\phi}^2}{2} + U(\phi), \\
\ddot{\phi} + 3 \frac{\dot{R}}{R} \phi + \frac{\partial U}{\partial \phi} &= 0.
\end{align*}
\]
Here a dot represents differentiation with respect to time. The choice of $U(\phi)$ is important and a particularly interesting choice with three free parameters is

$$U(\phi) = \lambda + \frac{m^2}{2\alpha^2} \sinh^2(\alpha\phi) + \frac{b}{2\alpha^2} \sinh(2\alpha\phi). \tag{7}$$

In the above expression $\lambda$ may be identified with a cosmological constant, $m^2 = \frac{\partial^2 U}{\partial \phi^2}|_{\phi=0}$ is a mass squared parameter, $b$ is a coupling constant and $\alpha^2 = \frac{3}{8}$. The Lagrangian giving the above equations of motion can be written as

$$L = -3\dot{R}\dot{R}^2 + 3kR + R^3[\dot{\phi}^2/2 - U(\phi)]. \tag{8}$$

This Lagrangian can be cast into a simple form for $k \neq 0$ describing an oscillator-ghost-oscillator system [7, 9]. Briefly, this is achieved by using the transformations

$$X = \frac{R^3}{2} \cosh(\alpha\phi)$$

and

$$Y = \frac{R^3}{2} \sinh(\alpha\phi),$$

which transform the term $R^3U(\phi) \cosh(\alpha\phi)$ into a quadratic form. Upon using a second transformation to eliminate the coupling term in the quadratic form, we arrive at new variables $u$ and $v$, which are linear combinations of $X$ and $Y$, in terms of which the Lagrangian takes on the simple form

$$L(u, v) = \frac{1}{2} \left[ (\dot{u}^2 - \omega_1^2 u^2) - (\dot{v}^2 - \omega_2^2 v^2) \right], \tag{9}$$

where $\omega_{1,2} = -3\lambda/4 + m^2/2 \mp \sqrt{m^4 - 4b^2}/2$. The classical solutions for $k \neq 0$ are given in [10].

The corresponding quantum cosmology for $k = 0$ is described by the WD equation written as

$$H\psi(u, v) = \left\{ -\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} + \omega_1^2 u^2 - \omega_2^2 v^2 \right\} \psi(u, v) = 0. \tag{10}$$

Alternatively, one may obtain a minisuperspace model described by the same WD equation but with equal frequencies by considering a closed Robertson-Walker universe with a vanishing cosmological constant and containing a conformally coupled scalar field [6]. A different model leading to the same WD equation with equal frequencies is obtained by considering a Kaluza-Klein cosmology with a negative cosmological constant described by the metric

$$g = -dt^2 + R^2(t) \frac{\sum dr^i dr^i}{(1 + kr^2/4)^2} + a^2(t) d\rho^2, \tag{11}$$

where $a(t)$ is the radius of the compactified space [8, 11]. The Lagrangian describing the above cosmology is

$$L = -\frac{1}{2}Ra\dot{R}^2 - \frac{1}{2}R^2\dot{\rho}a + \frac{1}{2}kRa - \frac{1}{6}\Lambda R^3 a, \tag{12}$$

where $\Lambda$ is the cosmological constant. By defining $\omega^2 = -\frac{2}{3}\Lambda$ and changing the variables as

$$u = \frac{1}{\sqrt{8}} \left[ R^2 - Ra - \frac{3k}{\Lambda} \right], \quad v = \frac{1}{\sqrt{8}} \left[ R^2 + Ra - \frac{3k}{\Lambda} \right], \tag{13}$$

$L$ takes on the form

$$L = \frac{1}{2} \left[ (\dot{u}^2 - \omega^2 u^2) - (\dot{v}^2 - \omega^2 v^2) \right]. \tag{14}$$

It is easily seen that the corresponding quantum cosmology is the same as [10] with equal frequencies. We therefore focus attention on solutions to equation (10).
3 Wave packets

Equation (10) is separable in the minisuperspace variables and a solution can be written as

$$\psi_{n_1,n_2}(u,v) = \alpha_{n_1}(u)\beta_{n_2}(v),$$

where

$$\alpha_n(u) = \left(\frac{\omega_1}{\pi}\right)^{1/4} \frac{H_n(\sqrt{\omega_1}u)}{\sqrt{2^n n!}} e^{-\omega_1 u^2/2},$$

$$\beta_n(v) = \left(\frac{\omega_2}{\pi}\right)^{1/4} \frac{H_n(\sqrt{\omega_2}v)}{\sqrt{2^n n!}} e^{-\omega_2 v^2/2},$$

Here $H_n(x)$ are Hermite polynomials, and the zero energy condition leads to

$$\left(n_1 + \frac{1}{2}\right)\omega_1 = \left(n_2 + \frac{1}{2}\right)\omega_2, \quad n_1, n_2 = 0, 1, 2, \ldots.$$  \hspace{1cm} (18)

The set $\{\psi_{n_1,n_2}(u,v)\}$ span the zero sector subspace of the Hilbert space of $L^2$ of measurable square integrable functions on $R^2$ with an inner product defined in the usual way giving

$$\int \psi_{n_1,n_2}(u,v)\psi_{n_1',n_2'}(u,v) du dv = \delta_{n_1,n_1'}\delta_{n_2,n_2'}.$$  \hspace{1cm} (19)

That is, the orthonormality and completeness of the basis functions follow from those of the Hermite polynomials.

We can construct a general wave packet as follows

$$\psi(u,v) = \sum_{n_1,n_2} \psi_{n_1,n_2}(u,v)\beta_{n_2}(v),$$

where the prime on the sum indicates summing over all values of $n_1$ and $n_2$ satisfying the constraint (18). As the signs of the kinetic terms in equation (10) indicate, we can take $v$ as playing the role of the scale factor and hence the initial condition on $\psi$ is specified by

$$\psi(u,0) = \sum_{n_1} \psi_{n_1}(u),$$

where the coefficients $\alpha_n$ are arbitrary and the double prime on the sum indicates that the sum runs only over those values of $n_1$ satisfying the constraint (18) with $n_2$ being even. The constraint on the evenness of $n_2$ is due to the fact that $\beta_{n_2}(0) = 0$ for odd values of $n_2$. We choose the coefficients $\alpha_n$ to be the same as those of the coherent states of a one dimensional simple harmonic oscillator, that is

$$c_n = e^{-\frac{1}{4}|\chi_0|^2} \frac{\chi_n^0}{\sqrt{2^n n!}},$$

where $\chi_0$ is an arbitrary complex number. Comparing the coefficients in equations (19,20) one finds for even values of $n_2$

$$\left(\frac{\omega_2}{\pi}\right)^{1/4} \frac{A_{n_1,n_2}}{\sqrt{2^{n_2} n_2!}} = \frac{c_{n_1}}{H_{n_2}(0)} = \frac{(n_2/2)!c_{n_1}}{(-1)^{n_2/2}n_2!},$$

where

$$c_{n_1} = e^{-\frac{1}{4}|\chi_0|^2} \frac{\chi_n^0}{\sqrt{2^n n!}}.$$
and $A_{n_1,n_2}$ are arbitrary for odd values of $n_2$. This arbitrariness is a consequence of not having specified $\partial \psi(u,v)/\partial v|_{v=0}$. The WD equation is a second order PDE, and to have a unique solution one has to specify both the wave function and its derivative at a given point. In the first reference in [6] the author has chosen $A_{n_1,n_2} = 0$ for odd values of $n_2$, which is equivalent to choosing $\partial \psi(u,v)/\partial v|_{v=0} = 0$. This might seem to be the only choice when considering equation (22). Here we argue that this is not the best or the ‘canonical’ choice. We have chosen $A_{n_1,n_2}$ to be nonzero and to have the same functional form for both even and odd values of $n_2$. This can be easily done using equation (23).

The classical paths corresponding to these solutions are the generalized Lissajous ellipsis which have the following parametric representation

$$u(t) = u_0 \cos(\omega_1 t - \theta_0), \quad v(t) = v_0 \sin(\omega_2 t), \quad (24)$$

where the zero energy condition demands $\omega_1 u_0 = \omega_2 v_0$, and $\theta_0$ is an arbitrary phase factor. The classical-quantum correspondence is established by the following equation

$$\chi_0 = \sqrt{\frac{\omega_1}{\omega_2}} u_0 e^{i\theta_0}. \quad (25)$$

Below we will consider several illustrative examples in order to compare our results with some of the previous works. Let us first consider the simplest case which is when $\omega_1 = \omega_2 = \omega$. Upon inspection of equations (17) through (19), we immediately recognize that, since $n_1 = n_2 = n$ and $H_n(0) = 0$ for odd values of $n$, firstly $A_{n,n}$ are not determined for odd values of $n$, and secondly

$$\psi(u,0) = \psi(-u,0), \quad (26)$$

$$\frac{\partial}{\partial v} \psi(u,v)|_{v=0} = - \frac{\partial}{\partial v} \psi(-u,v)|_{v=0}. \quad (27)$$

Therefore the initial state has to be symmetric and we choose it to be two symmetric Gaussians. However this is automatically taken into account by the restrictions imposed on the sum in equation (21) and the choice of coefficients given in equation (21). Also note that equation (27) is redundant due to the properties of the Hermite polynomials.

Figure 1 Shows the square of the wave packet $|\psi(u,v)|^2$ for $|\chi_0| = 12$ and $\theta_0 = 0$, summing over both even and odd values of $n$, and the contour plot of the same wave packet along with the classical path superimposed on it. In practice, in order to obtain a reasonable graphical representation, the minimum number of terms included in the sum, denoted by $n_{max}$, has to be of the order of $|\chi_0|^2$. As is apparent from these figures, the crest of the wave packet follows the classical path exactly. This is to be compared with figure 1 of the first reference in [6] which we reproduce here as figure 2 for the same value of $n_{max}$ as in figure 1. At this stage, due to the symmetry of the circle, the only advantage of our choice of the coefficients seems to be that the resulting wave packet is smoother. There is another advantage which will show up in the asymmetric case considered below.

One can easily interpolate between a circle and a line segment simply by changing the value of $\theta_0$ between zero and $\pm \pi/2$. Figure 3 shows the wave packet for $|\chi_0| = 12$ and $\theta_0 = 1$. This is
Figure 1: Left, the square of the wave packet $|\psi(u, v)|^2$ for $|\chi_0| = 12$ and $\theta_0 = 0$, $\omega_1 = \omega_2 = 1$ with $n_{max} = 130$ and right, the contour plot of the same figure with the classical path superimposed as the thick solid line.

Figure 2: Left, the square of the wave packet $|\psi(u, v)|^2$ for $|\chi_0| = 12$ and $\theta_0 = 0$, $\omega_1 = \omega_2 = 1$ with $n_{max} = 130$, summing only over even values of $n$ and right, the parametric plot of $|\psi(u, v)|^2$ along its crest showing rapid oscillations. The average frequency of these oscillations increases as $n_{max}$ increases.
Figure 3: Left, the square of the wave packet $|\psi(u,v)|^2$ for $|\chi_0| = 12$ and $\theta_0 = 1$, $\omega_1 = \omega_2 = 1$ with $n_{max} = 130$ and right, the contour plot of the same figure with the classical path superimposed as the thick solid line.

to be compared with figure 3 of the first reference in \[6\], where both wave packets with $\theta_0 = \pm 1$ are superimposed due to the choice $A_{n,n} = 0$ for odd values of $n$. This is not a desired result since in order to establish a classical-quantum correspondence we need to have a separate wave packet for each distinct classical path. At the classical level, a given set of initial conditions, e.g. specifying $u(0), v(0)$, uniquely determines a classical path. At the quantum level the initial conditions are specified for example by giving $\psi(u,0)$ and $\partial \psi(u,v)/\partial v|_{v=0}$, and this will uniquely determine a wave packet. Of course the initial conditions have to be consistent with the symmetries derived from the general structure of the solutions given by equation (19). In the present context, the first condition determines $A_{n,n}$ for even values of $n$, and the second the odd coefficients. Therefore the simultaneous appearance of two wave packets corresponding to two different classical paths is solely due to choosing $\partial \psi(u,v)/\partial v|_{v=0} = 0$ or equivalently setting $A_{n,n} = 0$ for odd values of $n$. This is in contrast to the interpretation given by the author in \[8\] where he relates the simultaneous appearance of two distinct branches to the superposition principle, and their only means of separation to the decoherence mechanism. As we have shown, for the class of problems discussed here, the use of the ansatz for the initial conditions given above would result in the selection of a unique branch without resorting to the decoherence mechanism.

As $\theta_0 \to \pm \pi/2$, the semi-minor axis of the ellipse goes to zero. The results are shown in figure 4. This configuration is to be compared with the approximate one obtained by adding a few terms with equal coefficients in \[8\].

Now we discuss the case with unequal frequency and to be concrete we give an example with $\omega_1 = 3\omega_2$. Then the constraint equation (18) gives $n_2 = 3n_1 + 1$. Therefore at $v = 0$ only the odd values of $n_1$ contribute. Hence we have

$$\psi(u,0) = -\psi(-u,0),$$

(28)
\[ \frac{\partial}{\partial v} \psi(u,v)
abla \bigg|_{v=0} = \frac{\partial}{\partial v} \psi(-u,v)
abla \bigg|_{v=0}. \] (29)

Again equation (29) is redundant and equation (28) is automatically taken into account by the restrictions imposed on the sum in equation (20). This together with the choice of the coefficients given in equation (21) gives two antisymmetric Gaussians. Only the coefficients \( A_{n_1,n_2} \) for odd values of \( n_1 \) are determined and those for even values of \( n_1 \) are fixed by the prescription given above. Figure 5 shows a plot of \( |\psi(u,v)|^2 \) for \( |\chi_0| = 6 \) and \( \theta_0 = 0 \). There are pronounced oscillations where there is an overlap between different branches of the wave packet due to the interference effect. This can be clearly seen from a parametric plot of \( |\psi(u,v)|^2 \) along the classical path similar to figure 2, which we do not show here. In figure 5 these oscillations are smoothed out and show up as the bump in the center of the figure. Also note that there is a good classical-quantum correspondence.

Let us next consider the case \( \theta_0 = \pi/2 \) whose wave packet is shown in figure 6. Note that there are pervasive pronounced oscillations due to the overlap. This configuration is to be compared with the approximate one obtained by adding a few terms with equal coefficients in \( \text{[7]} \). Moreover, the classical path presented in equation (33) of \( \text{[7]} \), describes an open curve which seems not to be correct. The correct parametric representation of the classical path which is a closed curve is given by equation (24).

4 Conclusions

We have described various classical cosmological models leading to a class of WD equations represented by equation (10). The general solution to this equation is a superposition of products of oscillator wave functions, as given in equation (19). We have argued that there exists a set of coefficients which produce wave packets with the following two desired properties.
Figure 5: Left, the square of the wave packet $|\psi(u,v)|^2$ for $|\chi_0| = 6$ and $\theta_0 = 0$, $\omega_1 = 3\omega_2 = 3$ with $n_{\text{max}} = 50$ and right, the contour plot of the same figure with the classical path superimposed as the thick solid line.

Figure 6: Left, the square of the wave packet $|\psi(u,v)|^2$ for $|\chi_0| = 6$ and $\theta_0 = \pi$, $\omega_1 = 3\omega_2 = 3$ with $n_{\text{max}} = 50$ and right, the contour plot of the same figure with the classical path superimposed as the thick solid line.
First, they possess a certain degree of smoothness, except when there is an overlap between different branches of the wave packet, where we expect some interference causing genuine pronounced oscillations. Second, there is acceptable classical-quantum correspondence. This correspondence consists of three conditions: The wave packet should have compact support centered around the classical path, the crest of the wave packet should follow as closely as possible the classical path, and to each distinct classical path there should correspond a unique wave packet with the above properties. The set of coefficients presented here as an ansatz is built from the coefficients of the coherent states as in ordinary quantum mechanics and coefficients derived from the functional form of $H_n(0)$ for even values of $n$. The resulting wave packets can be considered as coherent states in quantum cosmology and they possess all the aforementioned desired properties, and the classical paths are general Lissajous figures. We have shown these features explicitly in several examples. It is worth mentioning that, for the class of problems discussed here, the accomplishment of the last condition for classical-quantum correspondence by our choice of initial conditions shows that there is no need to employ decoherence mechanism to separate out wave packets corresponding to distinct classical paths. However, it is generally accepted that decoherence mechanism plays a major role in quantum-to-classical transition, see [12] for reviews. Although we have not shown the results explicitly here, we can report that as $|\chi_0|$ decreases the degree of classical-quantum correspondence diminishes. Also note that there is a difference between these coherent states and those of quantum mechanics in that the former are static.

We have also shown that there exists a continuous parameter $-\pi/2 < \theta_0 < \pi/2$, whose variation gives a continuous interpolation between wave packets or classical paths corresponding to different initial conditions. When $\theta_0 = 0$ we have the most symmetric configurations, i.e. loops which are symmetric about the line $u = 0$. When $\theta_0 = \pm \pi/2$ we have the most asymmetric configuration, i.e. curve segments.

This work is also related to the topic of initial conditions in the context of signature transition. For example, at the classical level there is a controversy on the value of $\dot{R}$ and $\dot{\phi}$ at the hypersurface of signature transition. The authors of reference [13] argue that these quantities need to be only continuous across the hypersurface, while in [14] it is insisted that in addition to the requirement of continuity, the values of both these quantities should be zero at the hypersurface. This choice corresponds to the most asymmetric case $\theta_0 = \pm \pi/2$, which gives curve segments as classical paths. We speculate that these are unlikely configurations due to their pronounced pervasive oscillations for $\omega_1/\omega_2 > 1$.

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