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Quantum dynamics beyond the Gaussian approximation

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The time-dependent quantum variational principle is emerging as an important means of studying quantum dynamics, particularly in early universe scenarios. To date all investigations have worked within a Gaussian framework. Here we present an improved method which is demonstrated to be superior to the Gaussian approach.

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I. INTRODUCTION

Early universe scenarios tend to be based on the evolution of scalar fields, either through their role as inflaton fields or as topological defects forming fields. A detailed understanding of the quantum evolution of these fields is important in order to fully describe their behavior during phase transition. This has recently been the focus of a great deal of attention. Its study relies on analyzing the quantum dynamics in real time. Guth and Pi [1] in one of the landmark papers in the field of inflation investigated the quantum mechanics of the scalar field in the new inflationary universe, looking in detail at the ''slow rollover'' transition. The idea of a ''slow rollover'' arises because the transition involves a scalar field ϕ which evolves slowly down its potential starting from some initial position where it is described by a well-defined wave function. The phase transition can be thought of as one where at very high temperatures the potential has a minimum at $\phi=0$, which becomes unstable as the temperature decreases, with the stable minima moving to a new larger value of $\phi=\pm\sigma$, say. As the universe cools the field remains close to $\phi=0$, slowly evolving towards its true vacuum value. The beginning of the phase transition is quantum mechanical in nature, yet the late time evolution of the scalar field is described by classical equations of motion. This assertion needs to be justified, as first addressed in [1]. Analyzing an exactly soluble linearized model, both in one-dimensional quantum mechanics and in quantum field theory of a single scalar field, it was discovered that the large-time behavior of the field in an unstable upside down harmonic oscillator potential is accurately described by ''classical physics.'' In the one-dimensional quantum-mechanical model the evolution of the wave function describing the particle in the potential is determined by the exactly solvable Schrödinger equation. The solution for the wave function is, not surprisingly, that of a Gaussian. The harmonic oscillator potential maintains the form of the initial Gaussian wave function.

In [2] the time-dependent variational method developed by Jackiw and Kerman [3] is used in the investigation of the behavior of a particle moving in a one-dimensional quantum mechanical with more realistic potentials (i.e., a double well potential), which have analogues both in the inflationary universe scenario and in models for the formation of topological defects. The important point that needs to be raised, and the motivation for this paper, is that in that work, and most subsequent work, the analysis is performed using a Gaussian trial wave function. The resultant equations of motion ob-

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tained through the variation of the effective action are the time-dependent Hartree-Fock (HF) equations. In [2] the authors argue that by comparison with the exact (numerical) solution the variational HF approximation accurately describes the process, and that the late time behavior of the evolution is approximately classical if described in terms of a suitably chosen small dimensionless coupling constant. We argue in this paper that it is straightforward to go beyond this Gaussian ansatz by expanding the wave function in a complete set of Hermite polynomials. In particular we find that just keeping the first and second order terms in the expansion leads to a dramatic improvement in the accuracy of the variational approach.

There are many reasons why it would be advantageous to go beyond the Gaussian approximation. If we have a potential which has degenerate minima, then it is impossible for a Gaussian wave packet to accurately describe the evolution of a scalar field during a phase transition. This is particularly relevant for calculations involving the formation of topological defects. For example, imagine we wish to understand the circumstances under which defects can be said to have formed and their distribution at formation. Recently in the context of vortices, there has been considerable attention paid to understanding the evolution of the scalar field responsible for their formation just after the quench transition [4]. One of the limitations of this interesting calculation is that it cannot accurately probe the nonlinear regions of the potential, hence it is only strictly valid just after the quench. In order to fully describe the formation process it is important to be able to probe the true vacuum of the potential.

In the context of our simple one-dimensional quantum mechanical system we hope to demonstrate that by extending the ansatz of the wave function to include the Hermite polynomials, then at little extra cost in complexity we can probe the nonlinear region of the potential in far greater detail than has previously been possible.

Another area where the nonlinearities of the theory need to be probed, is in the reheating calculations associated with inflation. As the inflaton field evolves down its potential, eventually it moves out of the ''slow roll'' regime as it descends into the true minima of the potential. The traditional picture is that in this region as the field oscillates about this minima then it decays through coherent oscillations and reheats the universe, restoring the radiation-dominated universe. Recently though, this picture has been questioned [5–7]. In order to fully probe this region of the potential, it is important that the ansatz adopted for the scalar field is valid in this region. It is our belief that the usual Hartree-Fock approximations are not sufficient here and need to be improved.

Use of the time-dependent variational principle of quantum mechanics is becoming more widespread. The method, first given by Dirac, involves the construction of an ''effective action''[1]

$$\Gamma = \int dt \langle \psi | i\partial_t - \hat{H} | \psi \rangle, \tag{1}$$

where $\partial_t \equiv \partial/\partial t$ and $\hat{H}$ is the Hamiltonian operator. Γ is then made stationary $\delta\Gamma = 0$ against variations of the state $\langle \psi |$ subject to the constraint $\langle \psi | \psi \rangle = 1$. Approximate[2] dynamics are obtained by positing a variational ansatz for the wave function that is a function of a small number of variables.

Central to the approach is the assumption that the ansatz for the variational wave function is ''close'' to the exact one; i.e., there are sufficient degrees of freedom for the wave function to accurately track the evolution of the system.

To date investigations have been restricted to the use of Gaussian ansätze since these are calculationally easy to handle. However, we shall argue that the Gaussian approach is of limited applicability and that results gained from it have a limited range of reliability.

II. THE VARIATIONAL PROCEDURE IN GENERALITY

In order to elucidate our later calculations it is useful to consider this construction in generality. Consider the variational effective action

$$\Gamma = \int dt \langle \psi | i\partial_t - \hat{H} | \psi \rangle. \tag{2}$$

Let us suppose the variational state to be a function of n real parameters v_i:

$$\Gamma = \int dt \frac{i}{2} \left(\langle \psi | \frac{\partial | \psi \rangle}{\partial v_i} - \frac{\partial \langle \psi |}{\partial v_i} | \psi \rangle \right) \dot{v}_i - \langle \psi | \hat{H} | \psi \rangle. \tag{3}$$

When the action is made stationary with respect to variation of these parameters we obtain the induced equations of motion

$$i \left[\frac{\partial \langle \psi |}{\partial v_j} \frac{\partial | \psi \rangle}{\partial v_i} - (i \leftrightarrow j) \right] \dot{v}_i - \frac{\partial}{\partial v_j} \langle \psi | \hat{H} | \psi \rangle = 0. \tag{4}$$

Schematically, this expression is of the form

$$A_{ij} \dot{v}_j - b_i = 0 \tag{5}$$

implying that in order that we are able to extract the equations of motion for the parameter v_j, the matrix A must be nonsingular throughout the evolution of the system.

III. IMPROVED WAVE FUNCTION

Before we give the expression for the improved wave function let us make the definition

$$u_n(x) := \left(\frac{\alpha}{\pi^{1/2} 2^n n!} \right)^{1/2} H_n(\alpha x) e^{-\alpha^2 x^2/2} \quad \alpha = (2G)^{-1/2}, \tag{6}$$

where $G(t)$ is real and H_n is the nth Hermite polynomial. We see that the u_n are a one parameter set of orthonormalized functions

[1]The connection of which to the usual effective action, or Gibbs free energy, is given in [3].

[2]It is not actually clear in what way the dynamics so obtained are approximate, an issue we will address in a later paper.

$$\int u_n(x)u_m(x)dx=\delta_{nm} \tag{7}$$

independent of the value of G. We may thus use the u_n as a basis for our variational wave function:

$$\psi(x,t)=Ne^{i\Pi x^2}\sum_{n=0}^{\infty} a_n u_n(x,t). \tag{8}$$

Here the a_n are time-dependent complex numbers, the other real variational parameters being Π and G which implicitly appear in the definition of the u_n. Normalization is achieved by the inclusion of a time-dependent N.

As it stands this represents no simplification. Our plan of action is therefore to truncate the expansion at some finite order and work consistently to that order. The zeroth-order approximation is simply the Gaussian, Hartree-Fock approximation.

As a test bed for our method we will consider the case of a particle moving in the potential considered by Cooper *et al.* [2], as this illustrates well the shortfalls of the Gaussian approach.

The potential we consider is of a double well,

$$V(x)=\frac{\lambda}{24}(x^2-a^2)^2, \tag{9}$$

with Gaussian initial conditions $G_0=\sqrt{3/2\lambda a^2}$, and a is the symmetry-breaking value for x.

To demonstrate the power of the method we will only include the first nontrivial term in the expansion. Since the potential and initial conditions are symmetric, the first nontrivial term involves u_2:

$$\psi=Ne^{i\Pi x^2}[u_0(x,t)+a_2u_2(x,t)]. \tag{10}$$

Even to this order we shall see that the improvement in the results over those of the Gaussian approach is impressive. We shall compare the results obtained using the improved equations of motion with the exact results obtained via numerical simulation.

IV. EQUATIONS OF MOTION

Working with a polar representation of $a_2(t)=Re^{i\theta}$, the equations of motion one obtains from Eq. (4) are

$$\dot{G}=4\Pi G-\frac{\sqrt{2}G^3s\lambda}{6R}, \tag{11}$$

$$\dot{\Pi}=\frac{1}{8G^2}-2\Pi^2+\frac{\lambda a^2}{12}-\frac{7G\lambda}{12}-\frac{\lambda\sqrt{2}cG}{24R}, \tag{12}$$

$$\dot{R}=s\lambda G^2\frac{(c+R^2c+2R\sqrt{2}+2R^3\sqrt{2})}{6R}, \tag{13}$$

$$\dot{\theta}=-\frac{\lambda G^2(4R^3\sqrt{2}c+2c^2R^2-2c^2+1-6R\sqrt{2}c-11R^2)}{12R^2}-\frac{1}{G}, \tag{14}$$

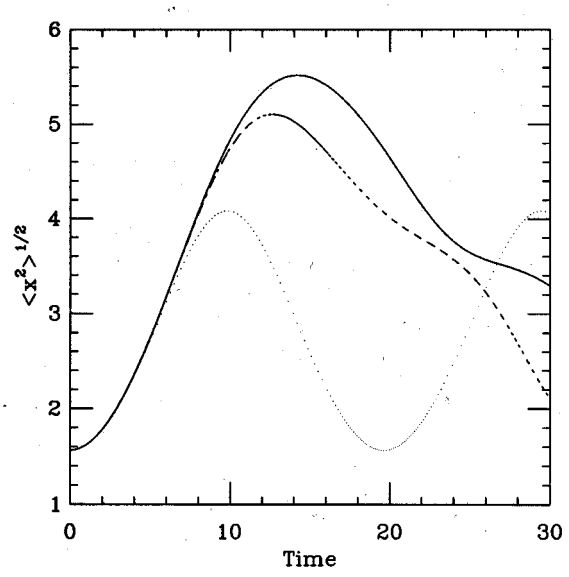

FIG. 1. Comparison of the methods for $a=5$.

where $s=\sin\theta$ and $c=\cos\theta$. The increase in complexity of the result over that of the Gaussian approach is more than compensated for by the increase in the accuracy of the results.

We notice that the improved equations of motion have within them terms familiar from the Gaussian approach. However, the HF equations of motion are not obtainable as a simple limit $a_2\to 0$ as the improved equations are singular in this limit. The origin of this singularity is as was outlined in Sec. II.

To assess the use of method we shall focus on the evolution of the quantity

$$\langle\hat{x}^2\rangle=\frac{G(1+5R^2+2\sqrt{2}Rc)}{1+R^2}. \tag{15}$$

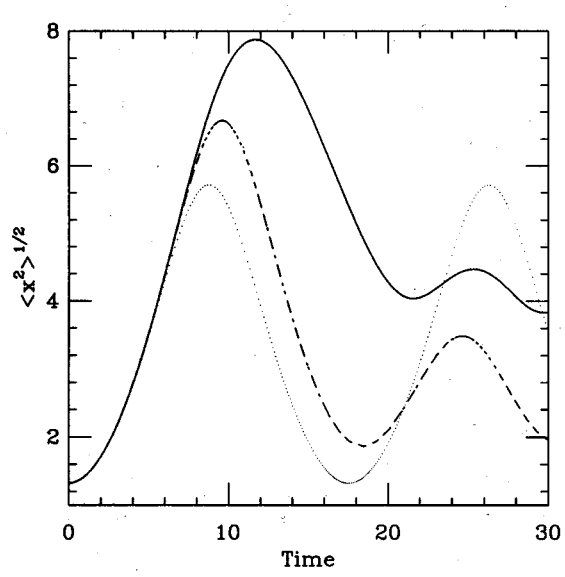

FIG. 2. Comparison of the methods for $a=7$.

V. INITIAL CONDITIONS

It is clear that the equations of motion are singular for the Gaussian initial conditions considered; since our aim is a comparison of the results of the improved method with those of Cooper *et al.*, we shall adopt the same initial conditions. This apparent problem is easily circumvented.

The rationale is to start the evolution of the system some short time after $t=0$. We solve the exact Schrödinger equation to first order and may then extract the values of R and θ, using these as the initial conditions in the variational equations of motion. In actuality the subsequent evolution of the system is rather insensitive to the initial conditions. This procedure leads us to take

$$R_0=\frac{\delta t\sqrt{2}(6+\lambda a^4 G_0)}{24}, \quad \theta_0=\frac{\pi}{2}. \tag{16}$$

VI. RESULTS AND CONCLUSIONS

The results of the above calculation are presented in Figs. 1 and 2. Plotted are the exact evolution of $\langle x^2\rangle$ found by numerical simulation (solid line), against the improved and Gaussian results (dashed and dotted lines, respectively) for the two values $a=5,7$. It is clear that the improved method furnishes us with a result considerably closer to the exact evolution than does the Gaussian. Also we see that the improved method samples regions of the potential much closer to the minima than does the HF, the so-called spinodal regions, suggesting that more information about the potential is being taken into account. The Gaussian wave function leads to a turning point of $\langle x^2\rangle$ at $2/3a^2$ [2], which provides an indication of where the ansatz breaks down. With the improved ansatz we find the turning point occurs typically at $\langle x^2\rangle\sim a^2$, demonstrating the significant increase in accuracy. Moreover, this approximate solution clearly probes the nonlinear region of the potential.

Behind this success is the crucial observation that the improved wave functions are capable of becoming bimodal in nature, something not open to the Gaussian ansatz. This means that we have a method of investigating the field evolution during a defect-forming transition and a first-order transition. These cases are currently being analyzed.

The ideal goal would be to apply the technique we have described to the field theory [8] case. Currently the Hartree-Fock approximation is generally adopted in variational calculations applied to the early universe [9]. Unfortunately the conversion from quantum mechanics to field theory is plagued with technical difficulties, which has so far prevented a successful implementation of the Hermite polynomial approach for the field theory case.

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