Quantum dynamics in a time-dependent variational approximation

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The time-dependent variational method, which in many-body theory leads to the Hartree-Fock approximation, is here tested in quantum-mechanical models inspired by the physics of the inflationary universe. Some remarks about field-theoretic applications are also made.

I. INTRODUCTION

Recently, as a result of new scenarios for the evolution of the early Universe[1,2] which involve quantum degrees of freedom, i.e., scalar fields, there has been revived interest in quantum dynamics in real time. Understanding quantum mechanics of the scalar field in the new inflationary universe is vital for a correct determination of the inflationary epoch's lifetime.[3] At present, an exact calculation of the field-theoretic quantum dynamics involves too many degrees of freedom to be reduced to a simple numerical computation, although attempts to find algorithms for that calculation are being studied. One obvious way to reduce the number of degrees of freedom is to use a variational method for determining approximate wave functionals in the Schrödinger picture.[4] A related method in the Heisenberg picture is to obtain the second Legendre transform of the generating functional, and to keep the lowest order in the coupling-constant 2-particle-irreducible graph.[5] Under certain circumstances, these fluctuation truncations are controllable approximations related to $1/N$ expansion, etc. In general, however, one does not have intuition about the domain of validity of such approximations. It is just this question that led us to this detailed study of quantum dynamics in double-well potentials as a prototype of the related field-theory problem. One of the nice features of the variational approximation is that the quantum theory is replaced by classical Lagrangian or Hamiltonian dynamics for the variational parameters $q(t)=\langle Q\rangle$ and $\hbar G(t)\equiv\langle Q^2\rangle-\langle Q\rangle^2$. Also, we are able to study in this approximation how well the static effective potential determines the dynamics of $q(t)$.

II. GENERAL FORMALISM

The time-dependent variational principle, posited by Dirac,[6] is an unconventional and novel approach for studying time-dependent quantum systems. In this section we shall review the subject following the work of Jackiw and Kerman.[4]

In classical physics, there are two variational principles. For time-dependent systems, Hamilton's least-action principle demands that the action

$$\Gamma=\int L\,dt=\int(P\dot{Q}-H)dt \tag{2.1}$$

be stationary. For time-independent systems, static configurations make the Hamiltonian stationary: $\partial H/\partial P=0$ and $\partial H/\partial Q=0$.

In quantum physics, the time-independent variational principle is also familiar. One demands that the expectation value of the Hamiltonian in a normalized state be stationary: $\delta\langle\psi|H|\psi\rangle=0,\langle\psi|\psi\rangle=1$. This provides a well-known derivation of the time-independent Schrödinger equation.

For time-dependent quantum systems, following Dirac, one considers time-dependent states $|\psi,t\rangle$ and requires that the time-integrated diagonal matrix element of $i\hbar\partial_t-H$,

$$\Gamma=\int dt\,\langle\psi,t|i\hbar\partial_t-H|\psi,t\rangle\ , \tag{2.2}$$

be stationary against variation of $|\psi,t\rangle$. Supplemented by appropriate boundary conditions, this provides a derivation of the time-dependent Schrödinger equation.

The quantity Γ is an effective action for a given system described by $|\psi,t\rangle$ and variation of Γ is the quantum analogue of Hamilton's principle. When a specific ansatz is made for the state $|\psi,t\rangle$, the time-dependent Hartree-Fock approximation emerges and this approach is widely used by quantum chemists[7] and nuclear physicists.[8]

In this paper we shall discuss one-dimensional quantum-mechanical systems with $H=(1/2m)P^2+V(Q)$. We are interested in the time evolution of a given initial Gaussian wave function in a time-dependent variational approximation. The effective action involves the diagonal matrix element of $i\hbar\partial_t-H$ in a trial wave function, which we take to be the most general Gaussian:

$$\langle Q|\psi,t\rangle_V=N\exp\left[-\frac{1}{2\hbar}(Q-q)^2B+\frac{i}{\hbar}p(Q-q)\right]. \tag{2.3}$$

Following Jackiw and Kerman, we parametrize the real and imaginary part of B as

$$B(t)=\tfrac{1}{2}G^{-1}(t)-2i\Pi(t)\ . \tag{2.4}$$

The normalization factor N is then $(2\pi\hbar G)^{-1/4}$. The real quantities $p(t)$, $q(t)$, $G(t)$, and $\Pi(t)$ are the variational parameters and we demand that their variations vanish at $t=\pm\infty$. The meaning of these parameters is seen from the equations

$$\langle Q\rangle_V = q(t)\ , \tag{2.5a}$$

$$\left\langle -i\hbar\frac{\partial}{\partial Q}\right\rangle_V = p(t)\ , \tag{2.5b}$$

$$\langle Q^2\rangle_V = q^2(t)+\hbar G(t)\ , \tag{2.5c}$$

$$\left\langle i\hbar\frac{\partial}{\partial t}\right\rangle_V = p\dot{q}+\hbar\Pi\dot{G}\ . \tag{2.5d}$$

From Eq. (2.5d), we notice that $\Pi(t)$ plays the role of the momentum canonically conjugate to $G(t)$. For potentials $V(Q)$ which are quartic in Q, the explicit form of Γ_V is

$$\Gamma_V(q,p,G,\Pi)=\int_{-\infty}^{\infty} dt\{p\dot{q}-H_{\rm cl}(q,p)+\hbar[\Pi\dot{G}-\tfrac{1}{2}GV^{(2)}(q)-\tfrac{1}{8}G^{-1}-2\Pi^2G]-\hbar^2\tfrac{1}{8}G^2V^{(4)}(q)\}\ , \tag{2.6}$$

where $H_{\rm cl}(q,p)=(1/2m)p^2+V(q)$ and $V^{(n)}(q)\equiv\partial^n V(q)/\partial q^n$. The four variational equations are then

$$\frac{\delta\Gamma_V}{\delta p}=0\rightarrow\dot{q}=\frac{1}{m}p\ , \tag{2.7a}$$

$$\frac{\delta\Gamma_V}{\delta\Pi}=0\rightarrow\dot{G}=4G\Pi\ , \tag{2.7b}$$

$$\frac{\delta\Gamma_V}{\delta q}=0\rightarrow\dot{p}=-V^{(1)}(q)-\tfrac{1}{2}\hbar GV^{(3)}(q)\ , \tag{2.7c}$$

$$\frac{\delta\Gamma_V}{\delta G}=0\rightarrow\dot{\Pi}$$

$$=\tfrac{1}{8}G^{-2}-2\Pi^2-\tfrac{1}{2}V^{(2)}(q)-\frac{\hbar}{4}V^{(4)}(q)G\ . \tag{2.7d}$$

We call the above "time-dependent Hartree-Fock" (HF) equations, because using the Gaussian wave function leads to the approximation in which all n-point expectation values are expressed in terms of one- and two-point functions.

From Eq. (2.6), the effective Hamiltonian, the energy of the system, in this approximation is given by

$$H_{\rm eff}=E=H_{\rm cl}(q,p)+\hbar(\tfrac{1}{2}GV^{(2)}+\tfrac{1}{8}G^{-1}+2\Pi^2G)$$
$$+\hbar^2\tfrac{1}{8}G^2V^{(4)}(q)\ , \tag{2.8}$$

and is a constant of motion. Also, by eliminating p and Π, we obtain the effective potential $V_{\rm eff}(q,G)$:

$$V_{\rm eff}(q,G)=V(q)+\hbar[\tfrac{1}{2}GV^{(2)}(q)+\tfrac{1}{8}G^{-1}]$$
$$+\hbar^2\tfrac{1}{8}G^2V^{(4)}(q)\ . \tag{2.9}$$

Extension of the time-dependent variational principle to quantum field theory in the functional Schrödinger picture is straightforward. We shall discuss this in Appendix A.

In this paper we shall apply Eqs. (2.7)–(2.9) to various quantum-mechanical problems to test the validity of the time-dependent HF approximation.

III. QUANTUM ROLL

The key feature of the new inflationary universe model[2] is a phase transition of a special type, often called a "slow rollover" transition. This name arises because the transition involves a scalar field ϕ which evolves slowly down a gentle hill in its potential diagram. In the very early Universe when the temperature was high, the potential has its minimum at $\phi=0$. As the temperature decreases, the minimum at $\phi=0$ becomes unstable or metastable and stable minima occur at some large values of $\phi=\pm\sigma$. Thus, as the Universe cools, the scalar field ϕ stays near $\phi=0$, and then eventually begins to roll down the hill slowly, toward the true minima. Although the beginning of this phase transition is quantum mechanical, the late-time behavior of the evolution is assumed to be governed by the classical equations of motion.

Recently, Guth and one of us[3] have carried out a detailed analysis to clarify the quantum theory of the "slow rollover" transition. An approximate, but exactly soluble linearized model was considered, both in one-dimensional quantum mechanics and in quantum field theory of a single scalar field. Among other things, an important result of this analysis is that the large-time behavior of a system in an unstable potential is accurately described by "classical physics." The one-dimensional quantum-mechanical toy model in which a particle is moving in the upside-down harmonic-oscillator potential,

$$V(Q)=-\tfrac{1}{2}kQ^2,\quad k>0\ , \tag{3.1}$$

was found to be particularly useful to demonstrate this result.

At $t=0$, a particle is described by a Gaussian wave function centered at $Q=0$. The evolution is then governed by the Schrödinger equation which is exactly soluble, and $\psi(Q,t)$ is precisely of the form given in Eqs. (2.3) and (2.4). Clearly, for $q(0)=p(0)=0$, $p(t)=q(t)=0$ for all t, and

$$\psi(Q,t)=(2\pi G\hbar)^{-1/4}\exp\left[-\frac{1}{2b^2}\tan(\alpha-i\omega t)Q^2\right]\ . \tag{3.2}$$

Therefore,

$$G^{-1}(t)=\frac{2\hbar}{b^2}\frac{\sin2\alpha}{\cos2\alpha+\cosh2\omega t}\ ,$$
$$\Pi(t)=\frac{\hbar}{2b^2}\frac{\sinh2\omega t}{\cos2\alpha+\cosh2\omega t}\ , \tag{3.3}$$

where $b^2=\hbar/\sqrt{mk}$ is a natural quantum-mechanical length scale of the problem and α is a real constant which is related to the width of the initial wave packet.[9]

For large times, the above wave function has the following information.

(i) The probability distribution for Q is given by

$$\langle Q^2\rangle\rightarrow\frac{1}{4}\frac{b^2}{\sin2\alpha}e^{2\omega t}\ ; \tag{3.4}$$

i.e., $\langle Q^2\rangle^{1/2}$ obeys a classical equation of motion with its smallest value when $\alpha=\pi/4$, i.e., when the initial width is given by

$$G_0\equiv G(0)=\frac{b^2}{2\hbar}\ . \tag{3.5}$$

This is due to the uncertainty principle.

(ii) Applications of momentum operator to ψ, at large times, yields

$$-ih\frac{\partial\psi}{\partial Q}=\left[\frac{i}{2}G^{-1}(t)+2\Pi(t)\right]Q\psi$$
$$=[\sqrt{mk}\ Q+O(e^{-2\omega t})]\psi\ . \tag{3.6}$$

Note that $\sqrt{mk}\,Q$ is the classical momentum $p_{\rm cl}=\sqrt{2m[E-V(Q)]}$ which would be attained by a *classical* particle at Q which rolled from rest at $Q=0$ with total energy $E=0$.

(iii) The commutator $[Q,P]$ is negligible if

$$\sqrt{mk}\ Q^2\gg\hbar,\ \text{i.e.,}\ \ Q^2\gg b^2\ , \tag{3.7a}$$

since

$$QP\psi=\sqrt{mk}\ Q^2\psi+O(e^{-2\omega t})\ ,$$
$$PQ\psi=\sqrt{mk}\ Q^2\psi-i\hbar\psi+O(e^{-2\omega t})\ . \tag{3.7b}$$

Note however that the wave function is definitely not sharply peaked about any particular classical trajectory. Rather the system is described by a classical probability distribution,

$$f(Q,P,t)=|\psi(Q,t)|^2\delta(P-p_{\rm cl})\ , \tag{3.8}$$

for large times. The function f obeys a classical evolution equation and the classical trajectories described by f can be parametrized as

$$Q(t)=Ce^{\omega t}\ , \tag{3.9}$$

where the random constant C is given by a Gaussian distribution.

In this section we shall study in the HF approximation the quantum-mechanical behavior of a particle moving in a more realistic potential of the form

$$V(Q)=\frac{\lambda}{24}(Q^2-a^2)^2\ . \tag{3.10}$$

As before, initially the particle is at the origin; $q(0)=p(0)=0$ and, therefore, $p(t)=q(t)=0$ for all t. We find, by comparison with the exact (numerical) solution, that the variational HF approximation accurately describes the process. Furthermore, we find that the late time behavior of the evolution is approximately classical if a dimensionless coupling constant, properly defined for this problem, is very small.

Our trial wave function for this problem is

$$\psi_V(Q,t)=(2\pi G)^{-1/4}\exp\{-\tfrac{1}{2}Q^2[\tfrac{1}{2}G^{-1}(t)$$
$$-2i\Pi(t)]\}\ . \tag{3.11}$$

(We have set $\hbar=1$.) A natural quantum-mechanical length scale b may be defined as

$$b^2\equiv\frac{1}{\sqrt{mk}},\quad k\equiv|V^{(2)}(0)|=\tfrac{1}{6}\lambda a^2\ . \tag{3.12}$$

We shall choose our initial width of the Gaussian to be

$$G_0=\tfrac{1}{2}b^2=\left[\frac{3}{2\lambda a^2}\right]^{1/2} \tag{3.13}$$

which in the upside-down harmonic oscillator leads to the smallest $\langle Q^2\rangle$ as we already have seen. This is necessary so that a "slow rollover" occurs before the particle reaches the potential minimum.

First, we discuss the general behavior of $G(t)$ in the HF approximation, where $G(t)$ can be found exactly. Conservation of energy gives, from Eqs. (2.7b) and (2.8),

$$E=\frac{\dot G^2(t)}{8G(t)}+\frac{\lambda}{8}G^2(t)+\frac{1}{8}G^{-1}(t)-\frac{\lambda a^2}{12}G(t)$$
$$=\frac{\dot G^2(t)}{8G(t)}+V_{\rm eff}(0,G(t))=V_{\rm eff}(0,G_0)\ . \tag{3.14}$$

The turning points of $G(t)$ are determined by

$$V_{\rm eff}(0,G(t))-V_{\rm eff}(0,G_0)$$
$$=\frac{[3G(t)-2a^2][2a^2\lambda G^2(t)-3]}{48a^2G(t)}=0\ . \tag{3.15}$$

We find that the maximum value of G is given by

$$G_m=\tfrac{2}{3}a^2\ , \tag{3.16}$$

so that $\sqrt{G}$ never gets to the minima at $Q=\pm a$, reflecting the failure of this approximation near the bottom of the two wells. However, as we shall see by direct comparison to the exact solution, the HF approximation is excellent for all $G<G_m$. It is clear that what is needed to describe the motion near $Q=\pm a$, is a trial wave function with two Gaussians.

We can obtain a closed expression for $t(G)$ for $G<G_m$:

$$t(G)=\int_{G_0}^{G}dG'\{8G'[E-V_{\rm eff}(0,G')]\}^{-1/2}$$
$$=\int_{G_0}^{G}dG'[(G_m-G')(G'-G_0)(G'+G_0)]^{1/2}\ . \tag{3.17}$$

This is an elliptic integral of the first kind.

Now we shall turn to our main interest, the large time behavior of the system. Unlike the upside-down harmonic-oscillator case whose potential always stays unstable, here "large" time is rather limited; it is some intermediate time before $(\langle Q^2\rangle)^{1/2}$ arrives near the minimum. In fact, in the HF approximation, "large time" is when $G(t)\lesssim\frac{2}{3}a^2$.

From Eqs. (3.7a) and (3.7b) we expect that the classical behavior may appear for $\langle Q^2\rangle\gg b^2$. This requires that

$$R\equiv\frac{b^2}{a^2}\ll1\rightarrow\frac{\sqrt{6}}{\sqrt{m\lambda}\,a^3}\ll1\ . \tag{3.18}$$

Equation (3.18) implies that for given m and a, λ must be large. One may define a dimensionless coupling constant for this problem in terms of the mass and of the

quantum-mechanical scale b as

$$\lambda' \equiv mb^6\lambda = \frac{6\sqrt{6}}{\sqrt{m\lambda}\,a^3} . \tag{3.19}$$

Then, $\lambda' \ll 1$ is equivalent to $R \ll 1$. The small value of λ' and R also implies that, in the harmonic approximation, the number of states N in the two wells at $Q = \pm a$ is large, indicating that classical behavior may be expected. In the harmonic approximation, N is given by

$$N - \frac{1}{2} = \frac{1}{4\sqrt{2}}\frac{1}{R} . \tag{3.20}$$

For our numerical calculation we have chosen $m = 1$, $a = 5$, and two values of λ; $\lambda = 3.84$ and $\lambda = 0.0123$.

For small dimensionless coupling constant, $\lambda' = 0.06$, which corresponds to $\lambda = 3.84$, we find the following.

(i) In Fig. 1 we compare $(\langle Q^2\rangle)^{1/2}$ in the exact solution to its HF approximation $\sqrt{G(t)}$. We find excellent agreement until $\sqrt{G}$ reaches its premature turning point at $a(\frac{2}{3})^{1/2}$. Despite this, a reasonable result for the oscillation time is obtained in the HF approximation. (The exact solution is obtained numerically in the Heisenberg picture.)

(ii) Classical behavior of $\langle Q^2\rangle$ in the late time: Since a classical particle with $Q(0) = P(0) = 0$, and therefore $E = (\lambda/24)a^4$, will stay at $Q = 0$, we did our computer experiment by placing the classical particle at $Q(0) = \sqrt{G_0}$ and compared the classical trajectory $Q_{\rm cl}(t)$ with the exact $(\langle Q^2\rangle)^{1/2}$ calculated in the Heisenberg picture. In Fig. 2 we find that for $1.5 < Q_{\rm cl} < 4$ (the first oscillation) the two are quite the same except for a shift of the origin. We have already seen in Fig. 1 that the HF approximation is excellent until $\sqrt{G}$ reaches $(\frac{2}{3}a)^{1/2} \approx 4.2$, and this implies that the classical behavior of $\sqrt{G}$ also appears in the HF approximation.

(iii) The classical behavior in Eq. (2.6) which is found in the upside-down harmonic oscillator is tested: We now find that

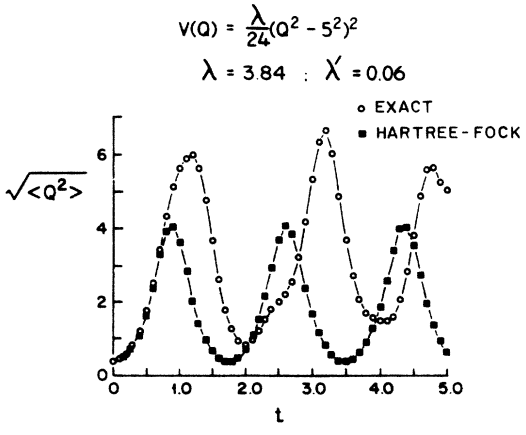

FIG. 1. Comparison of the exact quantum roll with the HF approximation for $\lambda = 3.84$; $\lambda' = 0.06$.

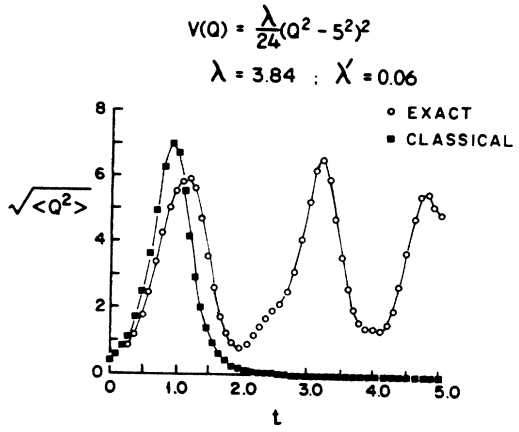

FIG. 2. Comparison of the exact quantum roll with a classical approximation for $\lambda = 3.84$; $\lambda' = 0.06$.

$$-i\frac{\partial\psi_V}{\partial Q} = \left[\frac{i}{2}G^{-1} + 2\Pi\right] Q\psi_V \approx 2\Pi Q\psi_V \tag{3.21}$$

and the ratio $2\Pi Q/p_{\rm cl}(Q)$, where

$$p_{\rm cl}(Q) = \sqrt{2[E - V(Q)]} = \left[\frac{\lambda}{12}\left[a^2 - \frac{Q^2}{2}\right]Q^2\right]^{1/2} ,$$

differs from unity by at most 20% for $1.5 < \sqrt{G} < 4$ in the HF approximation.

(iv) The question whether the commutator $[Q,P]$ is negligible is studied both in the HF approximation and in the exact calculation: In the HF approximation,

$$\langle QP\rangle_{\rm HF} = \frac{i}{2} + 2G\Pi \tag{3.22}$$

and we find that $G\Pi > 5$ for $1.75 < \sqrt{G} < 4$. In the exact calculation the real part of $\langle QP\rangle_{\rm exact} > 5$ for even larger range, i.e., $1.2 < (\langle Q^2\rangle)^{1/2} < 5.9$. Hence, from the above results, we see that for a small dimensionless coupling constant, $\lambda' \ll 1$ (or $\lambda > 1$) the late-time behavior of the system is approximately described by classical physics. As in the upside-down harmonic oscillator, our trial wave function ψ_V is not sharply peaked at any one classical trajectory. Therefore, the system is approximately described by a classical probability distribution function,

$$f(Q,P,t) = |\psi_V(Q,t)|^2 \delta(P - p_{\rm cl}) , \tag{3.23}$$

also in our variational time-dependent HF picture.

For a large dimensionless coupling constant, $\lambda' = 1.06$ (or $\lambda = 0.01$) we find that classical behavior does not appear in the HF approximation nor in the exact simulation: In the HF approximation $G\Pi < 1$ in Eq. (3.22), for all t, with its maximum value 0.71 at $\sqrt{G} = 3.3$. In the exact simulation, the real part of $\langle QP\rangle$ never exceeds 2. Hence, the real part of $\langle QP\rangle$ never becomes much larger than one in both cases and therefore the commutator $[Q,P]$ never becomes negligible. Figure 3 shows that the classical trajectory $Q(0) = \sqrt{G_0}$ and $E = (\lambda/24)a^4$, never follows the exact behavior $(\langle Q^2\rangle)^{1/2}$. A comparison of the

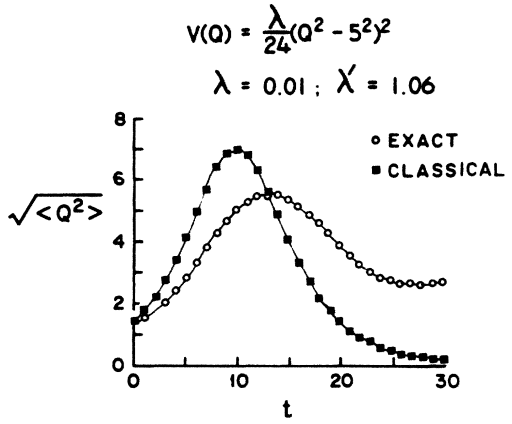

FIG. 3. Comparison of the exact quantum roll with a classical approximation for $\lambda=0.01$; $\lambda'=1.06$.

HF $\sqrt{G}$ and the exact $(\langle Q^2\rangle)^{1/2}$ is shown in Fig. 4: the HF approximation follows extremely closely the true quantum behavior up until its premature turning point. After that, $\sqrt{G}$ oscillates with too small oscillation frequency because it has a shorter distance to travel than the exact $(\langle Q^2\rangle)^{1/2}$. As mentioned earlier, this failure is due to the fact that the trial wave function is a *single* Gaussian.

IV. MOTION OF AN ANHARMONIC OSCILLATOR AND QUANTUM TUNNELING IN A DOUBLE-WELL POTENTIAL

As further tests of the validity of the time-dependent HF approximation we have studied motion of an anharmonic oscillator and quantum tunneling in a double-well potential.

A. Anharmonic oscillator

To see how well the HF method works in simple anharmonic oscillators, we studied the behavior of $\langle Q\rangle$ when

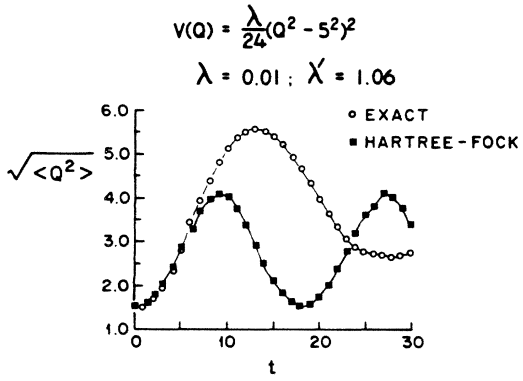

FIG. 4. Comparison of the exact quantum roll with the HF approximation for $\lambda=0.01$; $\lambda'=1.06$.

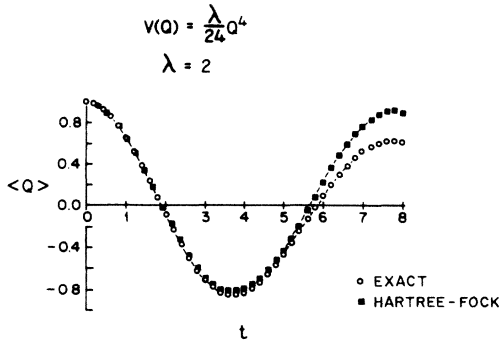

FIG. 5. Comparison of the exact $\langle Q\rangle$ with $q(t)$ in the HF approximation for an anharmonic oscillator.

we start with an initial Gaussian wave packet centered at $Q=a$, *not at the origin,* in a potential

$$V(Q)=\frac{\lambda}{24}Q^4 . \tag{4.1}$$

For simplicity, we choose $a=1$ and $\lambda=2$. The initial width of the Gaussian is again chosen as

$$G_0=\tfrac{1}{2}V^{(2)}(a) . \tag{4.2}$$

Our trial function is given by Eqs. (2.3) and (2.4) with $q(0)=1$, $p(0)=0$, $G(0)=\frac{1}{2}$, and $\Pi(0)=\frac{1}{2}$ as initial data.

In Fig. 5 we present a comparison of $\langle Q\rangle$ in the HF approximation with the exact numerical integration of the Heisenberg equations.[10] We find that during the first half of the oscillation cycle the two results are indistinguishable. Over many cycles, HF is reasonable good; it gives roughly the correct oscillation time although the detailed changes in the amplitude are different from the exact behavior.

B. Quantum tunneling

For potentials with two wells, two quite different behaviors are possible for an initial Gaussian wave packet located in one of the wells.[11] We may think that each well gives rise, in the harmonic approximation, to its own energy spectrum. Suppose the initial Gaussian localized in the left well is an approximate ground state. When its energy is almost degenerate with a level in the right well, an appreciable amount of probability leaks to the right well; we call this "on resonance." In this case, tunneling occurs and $\langle Q\rangle$ oscillates between the two wells. On the other hand, if the Gaussian's energy is not degenerate with any of the right well states, only a small amount of probability leaks through, and this is called "off resonance." Tunneling does not occur and $\langle Q\rangle$ oscillates between its initial value Q_0 and a value slightly larger than Q_0. We study this phenomenon in our time-dependent variational HF approximation.

First, we consider a potential of the form

$$V(Q)=\frac{\lambda}{24}Q^2(Q-a)^2 , \tag{4.3}$$

where the two wells at $Q=0$ and $Q=a$ are symmetric. Our initial wave function is chosen such that it is a ground state of the left well in the harmonic approximation:

$$\psi(Q,t=0)=\left[\frac{\omega_0}{\pi}\right]^{1/4}\exp(-\tfrac{1}{2}\omega_0 Q^2)\ , \tag{4.4}$$

where $\omega_0^2\equiv|V^{(2)}(0)|=(\lambda/12)a$. Again, we take our trial wave function as in Eqs. (2.3) and (2.4), with $q(0)=0$, $p(0)=0$, $G(0)=\frac{1}{2}\omega_0^{-1}$, and $\Pi(0)=0$. Since the potential has two symmetric wells, we expect "on resonance" tunneling process to occur. (A rough picture of this is described in Appendix B.) However, as we shall see, we find that the HF approximation cannot describe these tunneling processes.

One can explain this using the static effective potential. As we show later in this section, motion of $\langle Q\rangle$ in the HF approximation is roughly that of $q(t)$ governed by the classical dynamics of a potential $\tilde{V}_{\rm eff}(q)$ obtained by eliminating G in $V_{\rm eff}(q,G)$ via $(\partial V_{\rm eff}/\partial G)(q,G)=0$. From Eq. (2.9),

$$\tilde{V}_{\rm eff}(q)=\frac{\lambda}{24}q^2(q-a)^2+\tfrac{1}{2}G(q)V^{(2)}(q)+\frac{\lambda}{8}G^2(q)+\tfrac{1}{8}G^{-1}(q)\ , \tag{4.5}$$

where $G(q)$ is the solution of

$$2\lambda G^3+4V^{(2)}(q)G^2=1\ . \tag{4.6}$$

The behavior of $\tilde{V}_{\rm eff}(q)$ as λ changes from 1.92 to 123, for a fixed value $a=2$, is given in Figs. 6(a)–6(d). We see that $\tilde{V}_{\rm eff}(q)$ changes *as if* there were a phase transition. (Such a behavior was also found by Chang[12] in his study of $\lambda\phi^4$ field theory in two space-time dimension in the HF approximation.) For small values of λ, $\tilde{V}_{\rm eff}(q)$ is a single-well potential, but as λ increases there appears an energy barrier. We find that due to this energy barrier, classical dynamics of $q(t)$ in $\tilde{V}_{\rm eff}(q)$ in the HF approximation cannot describe tunneling processes.

In order to be more precise, consider the conserved energy of the system whose initial wave function is given by Eqs. (4.4). From Eq. (2.8), we have

$$E=\tfrac{1}{2}\omega_0+\frac{3}{8a^2}\ . \tag{4.7}$$

The second term in Eq. (4.7) is the HF correction to the harmonic approximation.

Our numerical study for $a=2$, shows the following: For $\lambda=1.92$, the energy of the system is larger than the energy barrier of the $V(Q)$ in Eq. (4.3): $E\simeq 0.49$ whereas $V(Q=1)=0.08$. There is no bound state in the two potential wells and we expect $\langle Q\rangle$ oscillates between $Q=0$ and $Q=2$ *without* tunneling. In Fig. 6(a), $\tilde{V}_{\rm eff}(q)$ is a single-well potential centered at $q=1$ and therefore $q(t)$ oscillates between $q=0$ and $q=2$. As shown in Fig. 7(a), the HF approximation agrees well with the exact answer.

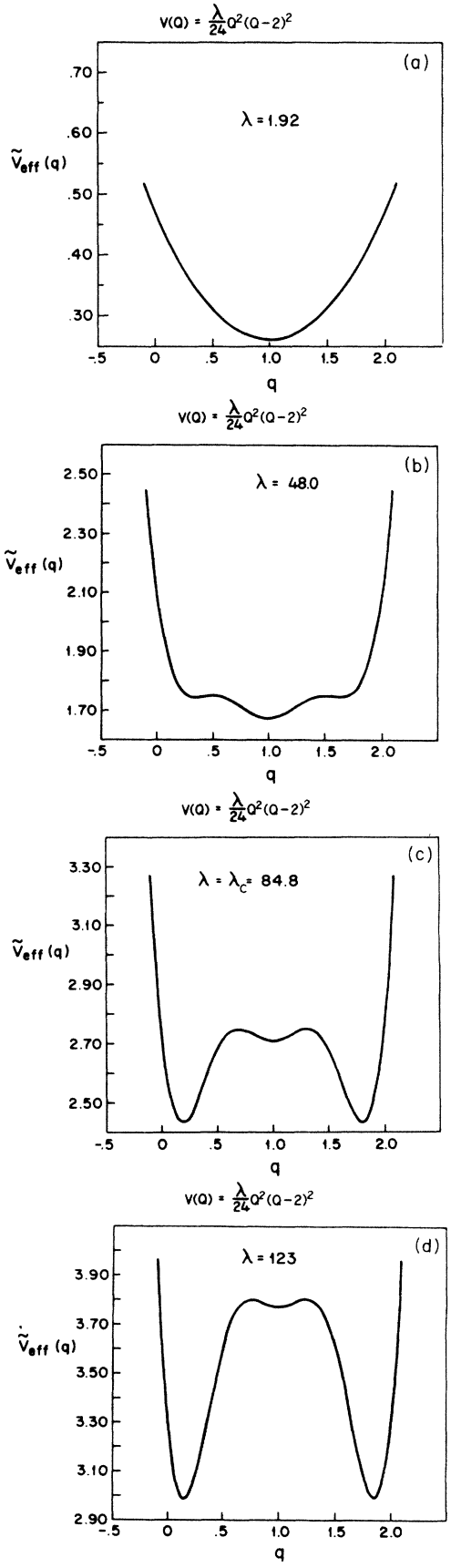

FIG. 6. A sequence of the HF effective potentials $\tilde{V}_{\rm eff}(q)$ for $V(Q)=(\lambda/24)Q^2(Q-2)^2$ as λ varies: (a) $\lambda=1.92$; (b) $\lambda=48$; (c) $\lambda=84.8$; (d) $\lambda=123$.

For $\lambda=48$, we still have $E\simeq 2.17 > V(Q=1)=2$. Figure 6(b) shows that $\tilde{V}_{\rm eff}(q)$ is still a single-well potential. The HF result is good for $t<2$, as shown in Fig. 7(b).

For $\lambda=\lambda_c=84.8$, we have $E\simeq 2.75 < V(Q=1)=3.53$, and our initial state is bounded in the left well. We expect in this case "on resonance" tunneling to occur. However, we see in Fig. 6(c) that for $\lambda=\lambda_c$, $\tilde{V}_{\rm eff}(q)$ has an energy barrier $\tilde{V}_{\rm eff}=E$. Classical dynamics of $q(t)$ barely describes the quantum tunneling. In Fig. 7(c) the HF approximation is already far from the exact answer.

For $\lambda>\lambda_c$, when the initial state is more deeply bounded in the left well, the energy barrier in $\tilde{V}_{\rm eff}(q)$ is larger than E [Fig. 6(d)] and the HF approximation cannot describe the tunneling phenomena; it gives only small oscillations inside the left well and q never enters the right well.

Next, we consider a case in which an initial Gaussian wave packet is in the left well of a potential $V(Q)=(\lambda/24)Q^2(Q-5)(Q-9)$ where two wells are *not* symmetric.[13] For such potentials, we expect off-resonance phenomenon, i.e., no tunneling.

HF behavior is given in Fig. 8, for $\lambda=\frac{5}{27}$. It is quite accurate for almost an entire oscillation which occurs in the left well. After that time, some probability which leaked into the right well destroys the accuracy of a single Gaussian picture.

Finally, we have studied the interesting question of how well the static effective potential describes the HF dynamics. Within the HF approximation, the equation for $\dot{p}$ is given by Eq. (2.7c):

$$\dot{p}(t)=-V^{(1)}(q)-\tfrac{1}{2}G(t)V^{(3)}(q)\ , \tag{4.8}$$

where $G(t)$ has its own dynamical equations, Eqs. (2.7b) and (2.7d). On the other hand, an approximate procedure, which is often used, eliminates G from $V_{\rm eff}(q,G)$ by solving $(\partial V_{\rm eff}/\partial G)(q,G)=0$, to give the static potential $\tilde{V}_{\rm eff}(q)\equiv\tilde{V}_{\rm eff}(q,G(q))$ and one posits the equation

$$\dot{\tilde{p}}(t)=-\frac{d\tilde{V}_{\rm eff}(q)}{dq}\ . \tag{4.9}$$

In Fig. 9(a), we compare Eqs. (4.8) and (4.9) in the case of $V(Q)=(\lambda/24)Q^2(Q-2)^2$ for $\lambda=48$, where the HF approximation works reasonably well. We see that the scatter of points of $\dot{p}$ are in a reasonably narrow band about $-d\tilde{V}_{\rm eff}/dq$. What is even more remarkable is that, as shown in Fig. 9(b), although the exact behavior of $\langle Q\rangle$ differs considerably from the HF $q(t)$, the time average of $\dot{p}_{\rm exact}(t)$ still follows the curve $-d\tilde{V}_{\rm eff}/dq$, although now the scatter is much wider. Thus, the effective potential $\tilde{V}_{\rm eff}(q)$ is a reasonable guide to the motion of $\langle Q\rangle$.

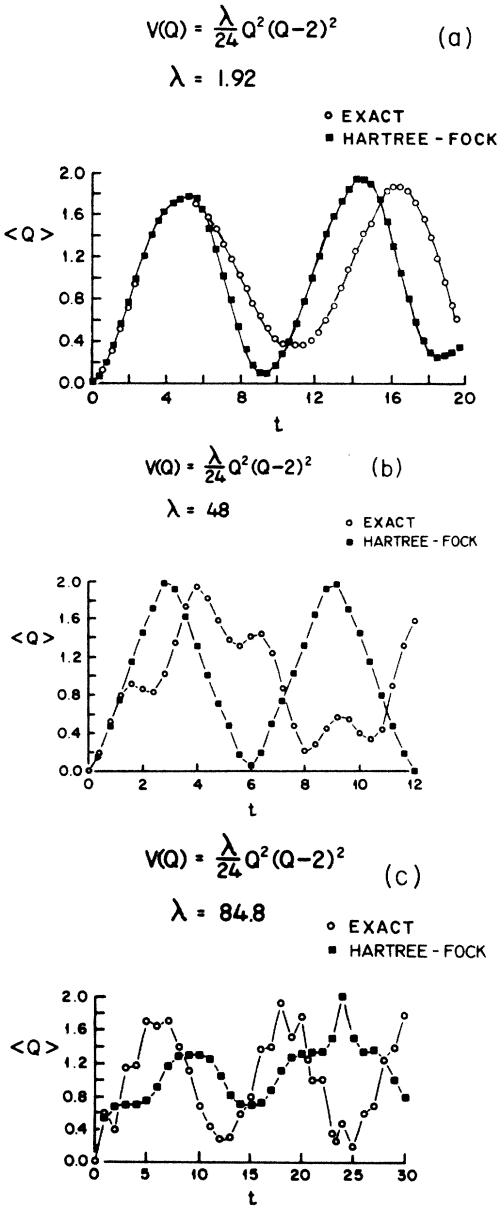

FIG. 7. Comparison of the exact $\langle Q\rangle$ and $q(t)$ in the HF approximation for various λ: (a) $\lambda=1.92$. The corresponding $\tilde{V}_{\rm eff}(q)$ is shown in Fig. 6(a). (b) $\lambda=48$. The corresponding $\tilde{V}_{\rm eff}(q)$ is shown in Fig. 6(b). (c) $\lambda=84.4$. The corresponding $\tilde{V}_{\rm eff}(q)$ is shown in Fig. 6(c).

V. CONCLUSION

The time-dependent variational HF approximation provides insight because it exhibits a simple physical picture

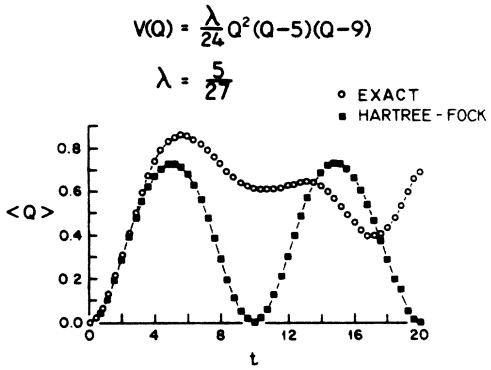

FIG. 8. Comparison of the exact $\langle Q\rangle$ and $q(t)$ in the HF approximation for $V(Q)=(\lambda/24)Q^2(Q-5)(Q-9)$; $\lambda=\frac{5}{27}$.

of the time evolution of a system in terms of a moving Gaussian with a time-dependent width and it is equivalent to the classical dynamics of two anharmonic oscillators q and G. The intuition we gain from this Schrödinger picture is far superior to the one from Green's functions and fluctuation expansions.

The variational HF approximation is a good approximation to the exact quantum dynamics whenever a single moving Gaussian has enough degrees of freedom to mimic the more complicated evolution of the exact wave function. We have found that the picture of a single expanding Gaussian is quite reasonable for the quantum-roll problem until $\sqrt{G}$ reaches near the bottom of the potential wells, and that the picture of a moving Gaussian is a good description of an anharmonic-oscillator problem.

However, whenever probability is expected to be localized at two different places at the same time, a single Gaussian is inadequate and the HF approximation fails.

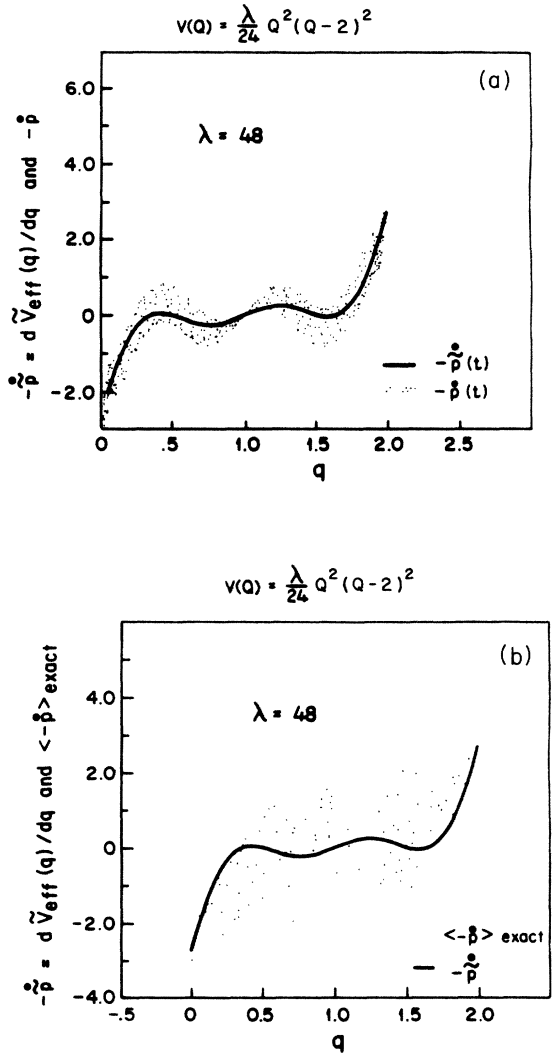

FIG. 9. (a) Comparison of $-\dot{p}(t)$ and $-\tilde{p}(t)=d\tilde{V}_{\rm eff}/dq$ in the HF approximation. (b) Comparison of the exact $\langle -\dot{p}(t)\rangle$ and $-\tilde{p}(t)=d\tilde{V}_{\rm eff}/dq$ in the HF approximation.

For example, in the case of the quantum roll, we found that the single Gaussian does not work near the bottom of the two wells, producing premature turning points for G. We have also found that the single Gaussian picture does not work in general for the on-resonance tunneling processes.

We expect that a variational calculation using a trial wave function with two or more Gaussian wave packets will have enough flexibility to model the quantum roll near the potential wells and the resonance tunneling processes (see Appendix B). It will be interesting to see if there is a simple Lagrangian description of the behavior of more complicated trial wave functions with two more more Gaussian wave packets.

In addition to the test of the HF approximation we have shown the validity of the assumption, which is crucial in the new inflationary Universe, that the late-time behavior of the quantum roll can be described by "classical physics." Also, we have shown that, within the HF approximation the dynamics of $q(t)=\langle Q\rangle$ is described reasonably well by the static effective potential $\tilde{V}_{\rm eff}(q,G(q))$.

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APPENDIX A: TIME-DEPENDENT VARIATIONAL METHOD FOR FIELD THEORY

We shall describe the time-dependent Hartree-Fock approximation in the functional Schrödinger picture for field theory. An abstract quantum-mechanical state $|\psi(t)\rangle$ is replaced by a wave functional $\Psi(\phi,t)$, which is a functional of a c-number field $\phi(x)$ at a fixed time:

$$|\psi(t)\rangle \rightarrow \Psi(\phi,t)\ . \tag{A1}$$

The action of the operator $\phi(x)$ on $|\psi(t)\rangle$ is realized by multiplying $\Psi(\phi,t)$ by $\phi(x)$:

$$\phi(x)\,|\psi(t)\rangle \rightarrow \phi(x)\Psi(\phi,t)\ . \tag{A2}$$

The action of the canonical momentum $\pi(x)$ is realized by functional differentiation

$$\pi(x)\,|\psi(t)\rangle \rightarrow -i\hbar\frac{\delta}{\delta\phi(x)}\Psi(\phi,t)\ . \tag{A3}$$

Then, the functional Schrödinger equation for a system is given by

$$i\hbar\frac{\partial\Psi(\phi,t)}{\partial t}=H\Psi(\phi,t)$$
$$=\int d^3x\left[-\frac{\hbar}{2}\frac{\delta^2}{\delta\phi^2(x)}+\tfrac{1}{2}(\nabla\phi)^2+V(\phi)\right]\Psi(\phi,t)\ . \tag{A4}$$

Now, we shall generalize the one-dimensional quantum-mechanical variational method to quantum field theory which has infinite degrees of freedom.

When we consider the problem of how a given initial state evolves with time, the effective action is given by

$$\Gamma=\int_{-\infty}^{\infty}dt\left\langle\psi\left|i\hbar\frac{\partial}{\partial t}-H\right|\psi\right\rangle \tag{A5}$$

and is stationary against an arbitrary variation of ψ.

For the time-dependent HF approximation, we take a Gaussian trial wave function which is the generalization of Eq. (2.3):

$$\Psi(\phi,t)_V=N\exp\left\{-\left[\int_{x,y}[\phi(\mathbf{x})-\hat{\phi}(\mathbf{x},t)]\left[\frac{G^{-1}}{4\hbar}(\mathbf{x},\mathbf{y},t)-i\frac{1}{\hbar}\Sigma(\mathbf{x},\mathbf{y},t)\right][\phi(\mathbf{y})-\hat{\phi}(\mathbf{y},t)]+\frac{i}{\hbar}\int_x\hat{\pi}(\mathbf{x},t)[\phi(\mathbf{x})-\hat{\phi}(\mathbf{x},t)]\right]\right\}, \tag{A6}$$

where N is the normalization state. The meaning of this wave function can be found by the following:

$$\langle\phi(\mathbf{x})\rangle_V=\hat{\phi}(\mathbf{x},t)\ , \tag{A7a}$$
$$\left\langle-i\hbar\frac{\delta}{\delta\phi(\mathbf{x})}\right\rangle_V=\hat{\pi}(\mathbf{x},t)\ , \tag{A7b}$$
$$\langle\phi(\mathbf{x})\phi(\mathbf{y})\rangle_V=\hat{\phi}(\mathbf{x},t)\hat{\phi}(\hat{y},t)+\hbar G(\mathbf{x},\mathbf{y},t)\ , \tag{A7c}$$
$$\left\langle i\hbar\frac{\partial}{\partial t}\right\rangle_V=\int_x\hat{\pi}(\mathbf{x},t)\dot{\hat{\phi}}(\mathbf{x},t)+\hbar\int_{x,y}\Sigma(\mathbf{x},\mathbf{y},t)\dot{G}(\mathbf{y},\mathbf{x},t)\ . \tag{A7d}$$

Ψ_V is Gaussian centered at $\hat{\phi}$ with width given by G. The conjugate momentum of $\hat{\phi}$ is $\hat{\pi}$ and Σ plays a role of the conjugate momentum of G. The variational parameters are $\hat{\phi}$, $\hat{\pi}$, G, and Σ.

The effective action in the trial state is then given by

$$\Gamma_V=\int dt\left[\int_x[\hat{\pi}\dot{\hat{\phi}}-\tfrac{1}{2}\hat{\pi}^2-\tfrac{1}{2}(\nabla\phi)^2-V(\hat{\phi})]+\hbar\left[\int_{x,y}(\Sigma\dot{G})-2\int_{x,y,z}\Sigma G\Sigma-\int_x[\tfrac{1}{8}G^{-1}(\mathbf{x},\mathbf{x},t)-\tfrac{1}{2}\nabla_x{}^2G(\mathbf{x},\mathbf{y},t)\,|_{\mathbf{x}=\mathbf{y}}+\tfrac{1}{2}V^{(2)}(\hat{\phi})G(\mathbf{x},\mathbf{x},t)]\right]-\hbar^2\tfrac{1}{8}V^{(4)}(\hat{\phi})\int_x G^2(\mathbf{x},\mathbf{x},t)\right]\ . \tag{A8}$$

Notice that the first integral is the familiar classical action. The variational equations are then

$$\frac{\delta\Gamma}{\delta\hat{\phi}(\mathbf{x},t)}=0\rightarrow\dot{\hat{\pi}}(\mathbf{x},t)=\nabla^2\hat{\phi}(\mathbf{x},t)-V^{(1)}(\hat{\phi})-\frac{\hbar}{2}G(\mathbf{x},\mathbf{x},t)V^{(3)}(\hat{\phi})\ , \tag{A9a}$$
$$\frac{\delta\Gamma}{\delta\hat{\pi}(\mathbf{x},t)}=0\rightarrow\hat{\pi}(\mathbf{x},t)=\dot{\hat{\phi}}(\mathbf{x},t)\ , \tag{A9b}$$
$$\frac{\delta\Gamma}{\delta G(\mathbf{x},\mathbf{y},t)}=0\rightarrow\dot{\Sigma}(\mathbf{x},\mathbf{y},t)+2\int_z\Sigma(\mathbf{x},\mathbf{z},t)\Sigma(\mathbf{z},\mathbf{y},t)$$
$$=\tfrac{1}{8}G^{-2}(\mathbf{x},\mathbf{y},t)+[\tfrac{1}{2}\nabla_x{}^2-\tfrac{1}{2}V^{(2)}(\hat{\phi})-\tfrac{1}{4}\hbar V^{(4)}(\hat{\phi})G(\mathbf{x},\mathbf{x},t)]\delta^3(\mathbf{x}-\mathbf{y})\ , \tag{A9c}$$
$$\frac{\delta\Gamma}{\delta\Sigma(\mathbf{x},\mathbf{y},t)}=0\rightarrow\dot{G}(\mathbf{x},\mathbf{y},t)=2\left[\int_z[G(\mathbf{x},\mathbf{z})\Sigma(\mathbf{z},\mathbf{y},t)+\Sigma(\mathbf{x},\mathbf{z},t)G(\mathbf{z},\mathbf{y},t)]\right]\ . \tag{A9d}$$

We shall now consider the quantum evolution of an initial Gaussian wave packet, in specific example where the potential is

$$V(\phi)=\frac{\lambda}{4}\left[\phi^2-\frac{\mu^2}{\lambda}\right]^2\ . \tag{A10}$$

Our initial data are given by $\hat{\phi}(\mathbf{x},0)=\hat{\pi}(\mathbf{x},0)=0$, $\Sigma(\mathbf{x},\mathbf{y},0)=\Sigma_0(\mathbf{x},\mathbf{y})$, and $G(\mathbf{x},\mathbf{y},0)=G_0(\mathbf{x},\mathbf{y})$. Then, translation invariance leads to simple HF equations in momentum space. G and Σ are functions of $(\mathbf{x}-\mathbf{y})$ and from Eqs. (A9c) and (A9d), we have

$$2\tilde{\Sigma}^2(\mathbf{k},t)+\dot{\tilde{\Sigma}}(\mathbf{k},t)=\tfrac{1}{8}\tilde{G}^{-2}(\mathbf{k},t)-\tfrac{1}{2}\Gamma\ , \tag{A11a}$$
$$\dot{\tilde{G}}=4\tilde{G}(\mathbf{k},t)\tilde{\Sigma}(\mathbf{k},t)\ , \tag{A11b}$$

where

$$\Gamma \equiv k^2-\mu^2+3\lambda \int \frac{d^3k}{(2\pi)^3}\tilde{G}(\mathbf{k},t) \tag{A11c}$$

and the tilde indicates Fourier transforms.

The above equations are as simple as one-dimensional quantum-mechanical equations except that they require renormalization. When we use the de Sitter background metric, they describe the dynamics involved in the "slow rollover" phase transition in the new inflationary universe, which occurs after the Universe supercools to a temperature much below the critical temperature when the effects of temperature are negligible. However, realistic initial values for G and Σ require information how the scalar fields behaves when the Universe cools from high temperatures.

APPENDIX B: TWO-STATE MODEL

For $V(x)=(\lambda/24)x^2(x-a)^2$, we have a variational trial function which is the sum of two Gaussians:

$$\Psi=\alpha\psi(x)+\beta\psi(x-a) , \tag{B1}$$

where

$$\psi(x)=\left[\frac{\omega}{\pi}\right]^{1/4} e^{-\omega x^2/2} .$$

Upon defining

$$\begin{aligned} A &= \int \psi(x)H\psi(x)dx = \int \psi(x-a)H\psi(x-a)dx , \\ B &= \int \psi(x)H\psi(x-a)dx = \int \psi(x-a)H\psi(x)dx , \\ C &= \int \psi(x)\psi(x-a)dx , \end{aligned} \tag{B2}$$

it follows that

$$E(\alpha,\beta)\equiv \frac{\langle \Psi \mid H \mid \Psi\rangle}{\langle \Psi \mid \Psi\rangle} = \frac{(\alpha^2+\beta^2)A+2\alpha\beta B}{\alpha^2+\beta^2+2\alpha\beta C} . \tag{B3}$$

If we choose for ω the harmonic-oscillator approximation $\omega^2=\omega_0{}^2=V^{(2)}(0)=V^{(2)}(a)=\lambda a^2/12$, then stationary states are obtained by minimizing with respect to α and β:

$$\frac{\partial E}{\partial \alpha}=\frac{\partial E}{\partial \beta}=0 \rightarrow \alpha=\pm\beta, \quad E_{\pm}=\frac{A\pm B}{1\pm C} . \tag{B4}$$

This variational calculation gives an approximate determination of the energy of the ground state $\Psi_+(x)$ and first excited state $\Psi_-(x)$. Observe that $\Psi(x)$ is just a linear combination of $\Psi_+(x)$ and $\Psi_-(x)$.

Consider the unnormalized approximate eigenfunctions

$$\begin{aligned} &\Psi_+(x)=\tfrac{1}{2}[\psi(x)+\psi(x-a)] , \\ &\langle \Psi_+ \mid H \mid \Psi_+\rangle = E_+\langle \Psi_+ \mid \Psi_+\rangle , \\ &\Psi_-(x)=\tfrac{1}{2}[\psi(x)-\psi(x-a)] , \\ &\langle \Psi_- \mid H \mid \Psi_-\rangle = E_-\langle \Psi_- \mid \Psi_-\rangle . \end{aligned} \tag{B5}$$

We have approximately

$$\begin{aligned} \Psi_+(x,t)&=\Psi_+(x)e^{-iE_+t} , \\ \Psi_-(x,t)&=\Psi_-(x)e^{-iE_-t} . \end{aligned} \tag{B6}$$

For our tunneling problem we choose

$$\Psi(x,t=0)=\Psi(x)=\Psi_+(x)+\Psi_-(x)$$

so approximately

$$\begin{aligned} \Psi(x,t)&=\Psi_+(x)e^{-iE_+t}+\Psi(x)e^{-iE_-t} \\ &=\tfrac{1}{2}e^{-iE_+t}\{[\psi(x)+\psi(x-a)] \\ &\quad +e^{-i\Delta Et}[\psi(x)-\psi(x-a)]\} , \end{aligned} \tag{B7}$$

where

$$\Delta E = E_- - E_+ + \frac{2(AC-B)}{(1-C^2)} . \tag{B8}$$

As a consequence

$$\begin{aligned} \Psi^{\dagger}(x,t)\Psi(x,t)&=\tfrac{1}{2}[\psi^2(x)(1+\cos\Delta Et) \\ &\quad +\psi^2(x-a)(1-\cos\Delta Et)] \\ &=\tfrac{1}{2}[\psi^2(x)+\psi^2(x-a)] \\ &\quad +\tfrac{1}{2}[\psi^2(x)-\psi^2(x-a)]\cos\Delta Et . \end{aligned} \tag{B9}$$

The time to tunnel is when $(\Delta E/2)T=\pi/2$ or

$$T=\frac{\pi}{\Delta E} . \tag{B10}$$

We also have

$$\langle x\rangle = a\sin^2\frac{\Delta Et}{2} , \tag{B11a}$$

$$\langle x^2\rangle = \frac{1}{2\omega}+a^2\sin^2\frac{\Delta Et}{2} , \tag{B11b}$$

and

$$\begin{aligned} A &= \frac{\omega}{4}+\frac{\lambda}{32\omega^2}+\frac{1}{48}\frac{a^2\lambda}{\omega} , \\ B &= e^{-\omega a^2/4}\left[\frac{\omega}{4}+\frac{\lambda}{32\omega^2}+\frac{\lambda a^2}{384}-\frac{\omega^2a^2}{8}-\frac{\lambda a^2}{96\omega}\right] , \\ C &= e^{-\omega a^2/4} . \end{aligned} \tag{B12}$$

If we choose $\omega=\omega_0$, then $\omega^2=\lambda a^2/12$ and we obtain

$$\begin{aligned} A &= \frac{\omega}{2}+\frac{3}{8a^2} , \\ B &= e^{-8V_0/\hbar\omega}\left[\frac{\omega}{8}+\frac{3}{a^2}-3V_0\right] , \\ C &= e^{-8V_0/\hbar\omega} , \end{aligned} \tag{B13}$$

where V_0 is the height of the barrier

$$V_0=V\left[\frac{a}{2}\right]=\frac{\lambda}{24}\left[\frac{a}{2}\right]^4 . \tag{B14}$$

We notice that A is just the Hartree-Fock energy (4.7) of the initial Gaussian wave packet. B and C are just the "instanton" corrections to the energy (B4). When ω is fixed at ω_0 we have

$$\Delta E=\frac{2(3V_0+3\hbar\omega/8)}{1-e^{-16V_0/\hbar\omega}}e^{-8V_0/\hbar\omega} . \tag{B15}$$

The oscillation time T predicted by this equation for the cases studied in this paper is of the correct order of magnitude.

One can improve on this approximation by allowing ω also to be a variational parameter. One then uses for ω, instead of ω_0, the solution of

$$\left.\frac{\partial E_\pm}{\partial\omega}\right|_{\omega=\omega_\pm}=0\rightarrow(384\omega_\pm{}^3-32a^2\lambda\omega_\pm-96\lambda)$$
$$\pm X_\pm[48a^4\omega_\pm{}^5-384a^2\omega_\pm{}^4+(768-a^6\lambda)\omega_\pm{}^3+12a^2\lambda\omega^2-16a^2\lambda\omega-192]$$
$$+X_\pm{}^2(384a^2\omega^4+384\omega^3+16a^2\lambda\omega-96\lambda)=0 , \tag{B16}$$

where

$$X_\pm=\exp\left[-\frac{a^2\omega_\pm}{4}\right] .$$

If there are many states in the well then

$$N=\frac{\lambda a^4}{384\hbar\omega}=\frac{V(a/2)}{\hbar\omega_0}=\frac{a^2\omega_0}{32\hbar} \tag{B17}$$

(actually, N should be replaced by $N-\frac{1}{2}$). This suggests an expansion in $1/N$ and e^{-N}. For large N one neglects the exponential and solves

$$12\omega^3-\lambda a^2\omega-3\lambda=0 .$$

Setting

$$\omega=\omega_0\left[1+\frac{\delta}{N}\right]$$

we obtain

$$\delta=\tfrac{3}{64} .$$

So when we can ignore e^{-8N} we have

$$\omega_\pm=\left[\frac{\lambda a^2}{12}\right]^{1/2}\left[1+\frac{3}{64N}+O\left[\frac{1}{N^2}\right]\right] . \tag{B18}$$

The two-state model gives a reasonable approximation for the tunneling time but gives a very smooth $x(t)$ which does not have the structure of the exact answer for the cases studied. We expect a time-dependent two-Gaussian model to work even better for the resonant tunneling calculation than this fixed position and width two-Gaussian model.

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