Nonperturbative approach for a time-dependent quantum mechanical system

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We present a variational method which uses a quartic exponential function as a trial wave function to describe time-dependent quantum mechanical systems. We introduce a new physical variable y which is appropriate to describe the shape of a wave packet, and calculate the effective action as a function of both the dispersion $\sqrt{\langle\hat{q}^2\rangle}$ and y. The effective potential successfully describes the transition of the system from the false vacuum to the true vacuum. The present method well describes the time evolution of the wave function of the system for a short period for the quantum roll problem and describes the long-time evolution up to 75% accuracy. These are shown in comparison with direct numerical computations of the wave function. We briefly discuss the large N behavior of the present approximation.

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The phase transition is one of the most important physical phenomena in nature and has a wide range of applications to condensed matter physics, particle physics, and cosmology. Most studies on this subject have been done in the framework of a quasistatic transition or using the Gaussian ansatz developed by Jackiw and Kerman [1]. There have been many attempts [2–4] to go beyond the Gaussian approximation. It is our purpose in this paper to go beyond the Gaussian approximation in two respects. First, we need a fully nonperturbative method to link the initial Gaussian packet (GP, false vacuum) to the symmetry broken degenerate vacuum state (true vacuum). Second, we try to find the relevant physical parameters which describe the symmetry breaking effectively.

In this paper, we consider a quantum mechanical model for time-dependent dynamics described by the potential

$$V(\hat{q},t)=\frac{\lambda}{24}[\hat{q}^2-k^2(t)]^2, \tag{1}$$

where $k^2(t)$ increases from a negative value to a positive number κ^2 asymptotically. The initial GP centered at $q=0$ cannot remain as Gaussian during the time evolution, but evolves to a packet centered around two minima of the potential as $k^2(t)$ approaches κ^2. For $\kappa^2\to\infty$, the new ground states are the linear sum or difference of two uncorrelated GPs centered at each minimum. In this case, the two ground states are degenerate.

The dispersion $\langle\hat{q}^2\rangle$ of a wave packet may describe the size of a GP or the distance between two packets of a double Gaussian packet (DGP). To discern the shapes (for example, GP or DGP) of wave packets of the same dispersion we introduce a dimensionless quantity y, which we call the ''shape factor,'' in addition to the dispersion (q^2):

$$q^2(t)\equiv\langle\hat{q}^2\rangle,\quad y(t)\equiv\frac{\langle\hat{q}^4\rangle}{\langle\hat{q}^2\rangle^2}. \tag{2}$$

A similar expectation value to y was calculated in Ref. [5] in relation to the new inflationary scenario. To illustrate the role of the y variable, consider a wave function that is a sum of two GPs of the same size. If $y=1$, the density of each GP is a delta function or the two GPs are infinitely far away so that no correlation exists between them, which provides the lower bound of $y(\geq 1)$. If the two GPs completely overlap, it corresponds to $y=3$, a single Gaussian packet. In between these two states, $1<y<3$, the two GPs are mixed and interfere with each other. For $y>3$, there are no separable packets, and the wave functions are better localized than the GP [6].

The effective action in the variational method [1] is given by

$$\Gamma=\int dt\langle\psi,t|i\partial_t-\hat{H}|\psi,t\rangle, \tag{3}$$

where $\hat{H}=\hat{p}^2/2m+V(\hat{q},t)$ and we use $\hbar=1$. In this paper we use the trial wave function

$$\langle Q|\psi,t\rangle=N^{-1}\exp\left[-\frac{1}{2}\left(\frac{1}{2\mu^2}+i\Pi\right)Q^4+\left(\frac{x}{\mu}+ip\right)Q^2\right], \tag{4}$$

which has both the DGP ($x\to\infty$) and the GP ($x\to-\infty$) limits, where we assume $\mu\geq 0$. In the static case, the double Gaussian approximation was used in Ref. [7], where a sum of two Gaussian functions is used as a trial wave function. However, it is difficult to generalize the double Gaussian method to the case for time-dependent systems. The normalization factor N can be determined by the following integral:

$$N^2=\int_{-\infty}^{\infty}dQ\exp\left(-\frac{Q^4}{2\mu^2}+\frac{2xQ^2}{\mu}\right)=\sqrt{\mu}f(x), \tag{5}$$

where $f(x)$ is given by [8]

$$f(x)=|x|^{1/2}e^{x^2}\frac{\pi}{\sqrt{2}}[I_{-1/4}(x^2)+\mathrm{sgn}(x)I_{1/4}(x^2)]. \tag{6}$$

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The dispersion and the ''shape factor'' for this wave function are

$$q^2(t)=\frac{\mu f'}{2f}, \quad y(t)=\frac{1+2xf'/f}{f'^2/(2f^2)}. \tag{7}$$

$y(x)$ is a nonincreasing function of x from 3 to 1, which makes the inverse function $x(y)$ be defined uniquely. We use y as a basic variable instead of x, because its range is bounded below by $y=1$ for any kind of wave packet [6] and it has definite physical meaning. The expectation values of other polynomials of $\hat{q}^2$ can be written in terms of these parameters.

With this trial wave function the effective action is given by

$$\Gamma=\int dt\left\{\frac{yq^4\dot{\Pi}}{2}-q^2\dot{p}-2y\left[y-\frac{y-3}{Y+1}\right]\frac{q^6\Pi^2}{m}-\frac{2q^2p^2}{m} +\frac{4yq^4\Pi p}{m}-U(q,y)\right\}, \tag{8}$$

where $Y(y)=2xf'/f=yf'^2/(2f^2)-1$ and the effective potential is

$$U(q,y)=\frac{V_F(y)}{8mq^2}+\langle V\rangle, \tag{9}$$

with the free potential V_F given by

$$V_F(y)=1+\frac{(3-y)(Y+1)}{y}. \tag{10}$$

This free potential, coming from the expectation value $\langle\hat{p}^2\rangle$, represents the effect of quantum mechanical uncertainty. The expectation value of the symmetric potential $V(\hat{q},t)=V_0(t)+(1/2)k(t)\hat{q}^2+[\lambda(t)/4!]\hat{q}^4+[c(t)/6!]\hat{q}^6+\cdots$ with respect to $|\psi,t\rangle$ is

$$\langle V\rangle=V_0(t)+\frac{k(t)}{2}q^2+\frac{\lambda(t)}{4!}yq^4+\frac{c(t)}{6!}y\left[y-\frac{y-3}{Y+1}\right]q^6 +\cdots. \tag{11}$$

From the action (8), we notice that Π and p are the momentum conjugates to $-yq^4/2$ and q^2, respectively.

Let us solve the Π and p equations first:

$$\frac{1}{8}\frac{d}{dt}\ln(yq^4)=-\left[1-\frac{y-3}{y(1+Y)}\right]\frac{yq^2\Pi}{m}+\frac{p}{m},$$

$$-\frac{1}{4}\frac{d}{dt}\ln q^2=\frac{yq^2\Pi}{m}-\frac{p}{m}. \tag{12}$$

Removing Π and p by Eq. (12) is just the Legendre transformation. Introducing the new variable η by $d\eta/dy\equiv D=(1/4)\sqrt{(1+Y/y(3-y))}$, we get a quite simple effective action in terms of η and q,

$$S=\int dt\left\{\frac{mq^2}{2}\dot{\eta}^2+\frac{m}{2}\dot{q}^2-U[q,y(\eta)]\right\}. \tag{13}$$

The dynamical equations of motion for q and η are given by

$$m\frac{d}{dt}[q^2\dot{\eta}]+\frac{1}{D}\left[\frac{V_F'(y)}{8mq^2}+\partial_y\langle V\rangle\right]=0, \tag{14}$$

$$m\ddot{q}-\frac{V_F}{4mq^3}+\partial_q\langle V\rangle=mq\dot{\eta}^2.$$

The free potential, $V_F(y)/8mq^2$ has an absolute minimum at $(y=3,\ q=\infty)$ and is positive definite. An interesting point here is that $y=3$, the GP, actually corresponds to $x=-\infty$. On the other hand, in the effective potential (10), $y=3$ is a regular point, which can be extended to larger values. This property of the effective potential implies that the trial wave function (4) is insufficient to give a full description of y dependence and we need a more general trial wave function for a complete quantum mechanical description which includes the range $y>3$. The generalization of the trial function to $|\langle Q|\bar{\psi},t\rangle|^2=\bar{N}^{-2}(1+|z|Q^2)^{-1}|\langle Q|\psi,t\rangle|^2$ may allow a full description of the y dependence, but is difficult to integrate. Instead, we use a patch for the region $y>3$,

$$\langle Q|\psi,t\rangle=N^{-1}\exp\left\{-\left(\frac{1}{4G}+i\Pi\right)Q^2+(-x+ip)|Q|\right\}, \quad y>3, \tag{15}$$

where we assume $x\geqslant 0$ and $G\geqslant 0$. The wave function is singular at the origin $Q=0$ due to the $|Q|$ term in the exponent. Hence we regard the absolute value as a small a limit of $\sqrt{Q^2+a^2}$. With this trial wave function, we have the same effective action as Eq. (13) with $D=\partial_y\alpha/2\alpha\sqrt{\alpha-1}$ $(y>3)$, and

$$V_F=\left[1+2z-\frac{2}{f}\sqrt{\frac{z}{\pi}}\right]\left(1+\frac{2}{f}\sqrt{\frac{z}{\pi}}\right) \quad \text{for } y>3, \tag{16}$$

where $z=2x^2G$, $f(z)=e^z(1-\mathrm{erf}\sqrt{z})$, and $\alpha=[1+2z-2\sqrt{z}/(\sqrt{\pi}f)]/2z[1/(\sqrt{\pi z}f)-1]^2$. The ''shape factor'' $y(z)$ monotonically increases from 3 to 6 as a function of z,

$$y(z)=\frac{3+12z+4z^2-2(5+2z)\sqrt{z}/(\sqrt{\pi}f)}{[1+2z-2\sqrt{z}/(\sqrt{\pi}f)]^2}. \tag{17}$$

As an example, let us consider the time evolution of an initial wave packet given by Eq. (4) with $(y=y_0, q=q_0)$ in the harmonic potential $s(t)\hat{q}^2/2$. The dynamics of y can be evaluated exactly from the elliptic integral

$$\int_{\eta_0}^{\eta}\frac{d\eta}{\sqrt{c^2-V_F[y(\eta)]}}=\pm\frac{1}{2m}\int_0^t dt'\frac{1}{q^2(t')}, \tag{18}$$

where $c^2=4m^2[\dot{\eta}(0)q^2(0)]^2+V_F[y(0)]$ is an integration constant. The equation of motion for q becomes

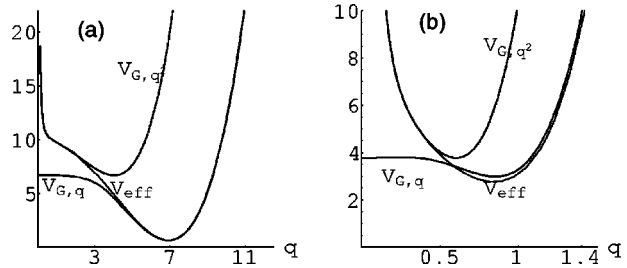

FIG. 1. The effective potential as a function of q for the parameters $\lambda=0.1$, $k=7$, $m=1$ (a), and $\lambda=123$, $k=1$, $m=1$ (b).

$$\ddot{q}(t)=-s(t)q(t)+\frac{2c^2-V_F(y)}{8m^2q^3(t)}. \tag{19}$$

If the system is potential-free $[s(t)=0]$, $\eta(t)$ asymptotically approaches a fixed value η_f and $q(t)$ asymptotically increases with a constant velocity determined by the energy conservation law. The allowed range, for constant $s(t)=s$, of q and y is also determined by the energy conservation law:

$$\frac{V_F(y)}{8mq^2}+\frac{1}{2}sq^2\leqslant E_{tot}=U(q_0,y_0). \tag{20}$$

Let us now consider the effective potential for the classical potential (1). The effective potential (9) naturally determines the true ground state with the condition

$$\partial_q U(q,y)=0=\partial_y U(q,y). \tag{21}$$

To see the behavior of the effective potential more clearly, we variationally determine y, and then write down the effective potential in q:

$$V_{eff}(q)\equiv U(q,y_v(q))=\frac{V_F(y_v(q))}{8mq^2}+\frac{\lambda}{24}[q^4y_v(q) -2k^2(t)q^2+k^4(t)], \tag{22}$$

where y_v means that we determine y by minimizing the effective potential with the condition $(\lambda/24)q^4=-V_F'(y_v)/mq^2$. In the static case this y_v value corresponds to the minimum position of the potential for a given q, which takes $y_v(0)=3$ and $y_v(\infty)=1$. We present figures (Fig. 1) of the effective potential (22) for two typical sets of parameters.

In these figures, $V_{eff}=U$, $V_{G,q}$, and V_{G,q^2} represent the effective potential (22), the Gaussian approximated effective potential for $\langle\hat{q}\rangle$, and the Gaussian approximated effective potential for $\langle\hat{q}^2\rangle$, respectively. Here, $V_{G,q}$ can be calculated from Eqs. (2.9) and (4.6) of Ref. [3] with a slight notational change $(q=\langle\hat{Q}\rangle)$ and V_{G,q^2} from Eq. (2.9) of Ref. [3] with $\langle\hat{Q}\rangle=0$ and $G\to q^2$. The effective potential V_{eff} is very close to V_{G,q^2} for $q<k/3$, and it becomes close to $V_{G,q}$ for $q>2k/3$. This clearly shows that the initial GP is divided into a DGP, with each packet of the DGP moving as if it is a free GP for large k. The value of $y_v[\sim 1+(3/\lambda mq^6)^{2/5}$ for $y_v\sim 1]$ is effectively 1 for the most of range of q if k is sufficiently large $[\gg(\lambda m)^{-1/6}]$, since the characteristic size of q is $O(k)$.

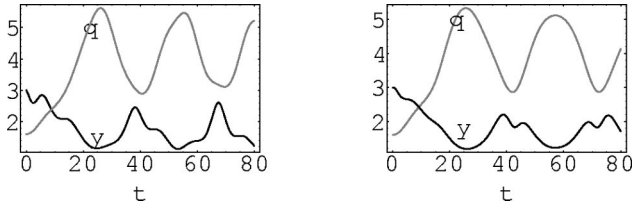

FIG. 2. Solution (left) of Eq. (14) and exact numerical time evolution by wave -function simulation (right) of $q(t)$ and $y(t)$. In this figure, we set $\lambda=0.0123$, $m=1$, $q_0=1.6$, and $y(0)=3$. $k(t)=t/3$ during $0\leqslant t\leqslant 15$ and remains constant afterward.

Let us explicitly describe the dynamics of an initial GP with $q=q_0$ $(\ll\kappa)$ for the time-dependent potential (1). Because of the transition [as $k(t)$ increases] y eventually goes to 1 for most of the dynamics. The potential energy difference $\triangle V=V_{eff}(q_0,y=1)-V_{eff}(q_0,y=3)>0$ and the presence of kinetic energy in y prevent q from reaching q_0. The time dependence of $k(t)$ decreases the total energy so that q oscillates near the true vacuum. We present, in Fig. 2, a solution of the differential equation (14) and its exact numerical solution for the case of $k(t)$ linearly increasing to a finite value for about a half period of q. In this example, we do not need the patching process by the wave function (15) since states with $y>3$ do not appear. To see the long-time behavior of the system, we present one more figure (Fig. 3). The main characteristic feature of the long-time behavior is the oscillation of the amplitude of short-time oscillation. The error of the oscillation period in Fig. 3 is about 25%. This error comes from the nonexactness of the variational wave function compared to the exact time evolution of the wave function.

As another example, let us consider the quenched transition potential with $k(t>0)=\kappa$ and $k(t<0)=0$. The discus-

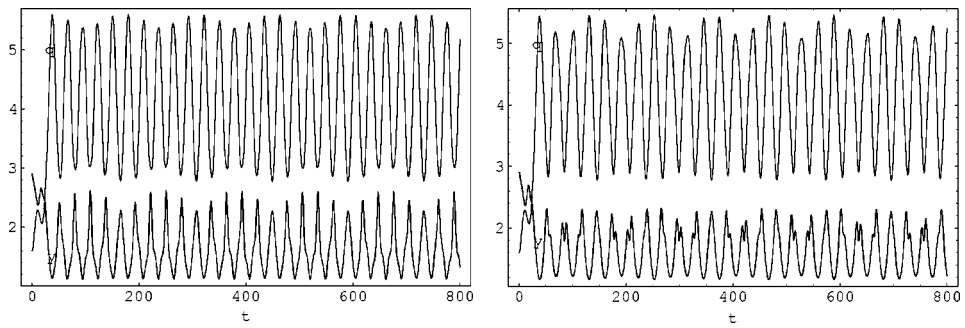

FIG. 3. Solution (left) of Eq. (14) and exact numerical time evolution by wave-function simulation (right) of $q(t)$ and $y(t)$. In this figure, we set $\lambda=0.0123$, $m=1$, $q_0=1.6$, and $y(0)=2.906$. $k(t)=t/3$ during $0\leqslant t\leqslant 30$ and remains constant afterward.

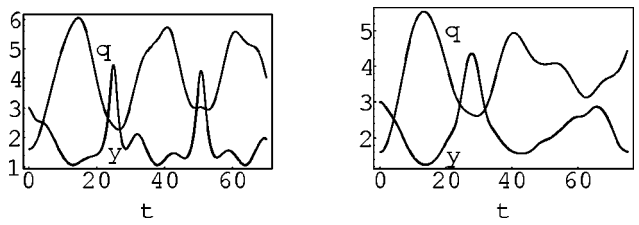

FIG. 4. Solution (left) of Eq. (14) and exact numerical time evolution (right) of $q(t)$ and $y(t)$ by wave-function simulation. In this figure, we set $\lambda=0.0123$, $\kappa=5$, $m=1$, $q_0=1.6$, and $y(0)=3$.

sion above for the time-dependent $k(t)$ transition also applies to the present example. We present a numerical solution of the differential equation (14) and its exact time evolution in Fig. 4. The state with large $y(>3)$ appears periodically. This means that we need the patching process (15) for the time evolution of this system. Comparing the two results in Fig. 4, one may notice the merits and the weakness of the present approach for the quenched transition. The present approach explains the periodic appearance of the large ''shape factor'' and well presents the period of its occurrence, but the details of the evolution are not exact. This discrepancy is related to the ''patched'' trial wave function (4) and (15) at $y=3$. We have chosen this artificial patching method because of its simplicity. A better approach may be to include the excited states of Eq. (4) without introducing the patching (15). One of the excited states $\langle Q|\psi_2,t\rangle=(y-1)^{-1/2}(Q^2/q^2(t)-1)\times\langle Q|\psi,t\rangle$ is an orthonormal wave function to $\langle Q|\psi,t\rangle$. Because of the symmetry of the potential (1), the odd function of q cannot contribute to the evolution. One may try the variational method by using the following trial wave function:

$$\langle Q|\overline{\psi},t\rangle=\overline{N}^{-1}[\langle Q|\psi,t\rangle+z\langle Q|\psi_2,t\rangle], \tag{23}$$

where z is a complex valued function of time and the normalization factor is $\overline{N}^2=1+|z|^2$. This wave function naturally includes the regions with $y>3$ due to the contribution of the excited state. In this sense, the appearance of a large ''shape factor'' (>3) is the signal for the contribution of excited states in the time evolution of the systems. Generally, the accuracy of the approximation (4) increases as the potential varies slowly. We applied the present method to the case of scalar ϕ^4 field theory in Ref. [9], and it would be interesting to apply more realistic quantum mechanical systems in a second order phase transition.

Another point we need to speculate is the large N limit. It was shown that the large N wave function satisfies [10]

$$i\frac{\partial\Phi(z,\tau)}{\partial\tau}=\left[-\frac{1}{2N^2}\frac{\partial^2}{\partial z^2}+u(z,N)\right]\Phi(z,\tau), \tag{24}$$

where $\tau=Nt$, $r^2\equiv\Sigma_{k=1}^{N}x_k^2=Nz^2$, and $u(z,N)=(N-1)(N-3)/8N^2z^2+(g/8)(z^2-z_0^2)^2$. The present approximation for a symmetric state is given by

$$\Gamma=\int d\tau\langle\psi,\tau|i\partial_\tau-\frac{1}{2N^2}\Pi^2-u(z,N)|\psi,\tau\rangle. \tag{25}$$

This is the same as Eq. (3) with the change of parameters $t,Q,m,V(Q,t)\rightarrow\tau,z,N^2,u(z,N)$. With the use of the trial wave function (4) in Eq. (25) the expectation value of $(1/2N^2)\Pi^2$ is given by

$$2y\left[y-\frac{y-3}{Y+1}\right]\frac{q^6\Pi^2}{N^2}+\frac{2q^2p^2}{N^2}-\frac{4yq^4\Pi p}{N^2}+\frac{V_F(y)}{8N^2}, \tag{26}$$

where the first three terms in Eq. (26) are $O(1)$, and in the large N limit the quantum mechanical effects on the potential $V_F/(y)8N^2$ effectively vanish as $O(1/N^2)$. In the absence of this quantum mechanical term, the equation of motion in the large N limit for the present quartic exponential approximation with $y=1$ is the same as that of the Gaussian approximation centered at $z\neq0$. Since the Gaussian approximation was proven to be the same as the large N approximation [11], the present approximation is equivalent to the large N approximation for $N\rightarrow\infty$.

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