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Semiclassical methods at finite temperature

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Semiclassical path-integral methods are applied to the quantum-mechanical double-well potential at finite temperature. When all parameters are fixed and $\hbar \to 0$ the quantum tunneling transitions which maintain the symmetry at zero temperature are absent. Classical thermal fluctuations, however, give transitions which partially disorder the system.

I. INTRODUCTION

We apply semiclassical path-integral methods to the finite-temperature quantum-mechanical double-well potential. At zero temperature quantum-mechanical tunneling transitions maintain the symmetry. At finite temperature classical thermal fluctuations as well as quantum fluctuations disorder the system. This motivates us to study the limit in which all parameters of the problem (the inverse temperature $\beta = 1/kT$, the coupling constants, and the real or imaginary time of the correlation functions) are fixed and $\hbar$ is taken to zero. The goal is to give a perturbation-theory loop expansion in which the first term contains the full classical result. (A high-temperature expansion would lead off with a term which is the high-temperature limit of the classical result.)

Previous finite-temperature investigations have been carried out for weak coupling and for large N, particularly in connection with the restoration of spontaneously broken symmetries.[1] Some low-temperature semiclassical estimates of the partition function have been performed in one- and two-dimensional models.[2,3] In this paper we are examining a system whose symmetry is already manifest at zero temperature. Since this system admits no instantons above a certain temperature,[2,4] we were led to investigate the symmetry properties for temperatures above this value. As is discussed below, we do this by studying the real-time finite-temperature correlation function. We find that at a fixed time in a small-$\hbar$ approximation the correlation function is a decreasing function of increasing temperature. From this we conclude that the disorder associated (in analogy with a spin system) with the symmetry at zero temperature increases as the temperature is raised.

In Sec. II we compute a semiclassical expansion for the partition function $Z = \mathrm{Tr}\, e^{-\beta H}$. Z is represented as a Euclidean functional integral over paths $x(\tau)$ for which $x(0) = x(\beta\hbar)$. An expansion about a stationary path of the Euclidean action, a path whose end point is constrained, followed by an integration over the end point gives a loop expansion in which the first term contains the full classical expression Z_{cl}. Had we perturbed about a constant stationary point, we would have found an expansion in the anharmonic terms of the potential, an expansion whose leading term is a harmonic approximation, not the full classical result.

In Sec. III we compute a semiclassical expansion of the finite-temperature Euclidean correlation function[5]

$$\mathcal{C}\left(\frac{\tau}{\hbar}\right) = \frac{1}{Z} \mathrm{Tr}\, e^{-\beta H} x(\tau) x(0) , \tag{1.1}$$

where

$$x(\tau) = e^{H\tau/\hbar} x(0) e^{-H\tau/\hbar}$$

and

$$0 \leqslant \tau \leqslant \beta\hbar .$$

The constrained-end-point method of Sec. II is used. We find the expansion to be systematic if we introduce a new variable $\sigma \equiv \tau/\hbar$ and express the correlation function (1.1) in terms of σ. The leading term, however, cannot be used to obtain a small-$\hbar$ approximation to the real-time correlation function $C(t)$ since that would involve the continuation[5]

$$\sigma \to \frac{it}{\hbar} . \tag{1.2}$$

In order to regain a simple systematic expansion using semiclassical methods, we calculate in Sec. IV the real-time correlation function directly from a functional integral representation. This involves a product of three path integrals whose semiclassical approximation is shown to include the complete classical answer $C_{\mathrm{cl}}(t)$ in the limit t fixed, $\hbar \to 0$.

In Sec. V the classical correlation function $C_{\rm cl}(t)$ is computed for the double well in the limit $t\to\infty$. The Hamiltonian is

$$H=\tfrac{1}{2}p^2+V(x),\quad V(x)=\frac{g^2}{4}\left(x^2-\frac{\omega^2}{g^2}\right)^2, \tag{1.3}$$

and

$$\lim_{t\to\infty} C_{\rm cl}(t)=\frac{\omega^2}{g^2}c\left(\frac{\beta\omega^4}{g^2}\right). \tag{1.4}$$

The function $c(\beta\omega^4/g^2)$ is roughly the ratio of the volume of phase space with energy less than the barrier height $\omega^4/4g^2$ to that with energy less than $1/\beta$,

$$c\left(\frac{\beta\omega^4}{g^2}\right)\to 0 \text{ as } \beta\to 0.$$

We now discuss the role of the symmetry $x\to -x$ in this problem and the relevance of the classical calculation for the quantum problem. At zero temperature it is useful to consider

$$\lim_{\hbar\to 0}\lim_{\tau\to\infty}\mathcal{C}(\tau/\hbar)\big|_{\beta=\infty}. \tag{1.5}$$

Polyakov[6] shows that the contribution of the kink solutions to the Euclidean path integral restores the symmetry and (1.5) is zero. The order of the limits is crucial. If the order were reversed,

$$\lim_{\tau\to\infty}\lim_{\hbar\to 0}\sum_n e^{-E_n\tau/\hbar}|\langle n|x|0\rangle|^2,$$

the result would be nonzero. At fixed finite temperature, $0\leq\tau\leq\beta\hbar$ and the $\tau\to\infty$ limit is not available. We thus investigate the real-time finite-temperature correlation function. It is an almost periodic function. $C(t)$ does not have the simple structure at large t that $\mathcal{C}(\tau/\hbar)$ has a zero temperature and large τ.

Nevertheless, we shall make some qualitative observations. Equation (1.4) reflects the classical fact that at any finite temperature some fraction of the particles in an ensemble cannot have enough energy to go over the barrier and thus they give a positive contribution to the correlation function. Quantum tunneling does not affect this result until t is of the order of the typical tunneling time t_T for the ensemble. This tunneling time includes a factor $e^{S/\hbar}$ where S is some positive constant. However, since $C(t)$ is an almost periodic function it is difficult to estimate in this large time region.

In Sec. VI we suggest some paths that may be important in this large t region. In our study of the symmetry behavior of the finite-temperature quantum theory, however, we restrict ourselves to the limit fixed t and $\hbar\to 0$. In this region of time tunneling effects are absent, and the quantum correlation function is within $O(\hbar)$ of $C_{\rm cl}(t)$.

In the four-dimensional zero-temperature Yang-Mills system, it has been suggested that instantons are responsible for the restoration of a symmetry which results in quark confinement.[6] Thus one would be led naturally to study the symmetry properties at finite temperature to investigate quark liberation.[7]

Although no attempt is made to study such an ambitious system in this paper, we remark that our one-dimensional investigation was in part motivated by such considerations and may serve as a first arena in which to understand these ideas.

II. THE PARTITION FUNCTION

The partition function Z can be expressed as a path integral over periodic paths:

$$Z=N\int_{\substack{\text{all paths}\\ x(0)=x(\beta\hbar)}} Dx\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar}d\tau\left(\frac{\dot{x}^2}{2}+V(x)\right)\right]. \tag{2.1}$$

The normalization factor N is independent of the potential and depends on the normalization of the measure Dx; to estimate (2.1) by a saddle-point method we look for the minima of $I[x]\equiv\int_0^{\beta\hbar}d\tau \times[\dot{x}^2/2+V(x)]$ subject to the conditions $x(0)=x(\beta\hbar)$. That is to say, we must find solutions to the classical equation $\ddot{x}_{\rm cl}=V'(x_{\rm cl})$ with $\dot{x}(0)=\dot{x}(\beta\hbar)$.[8]

An expansion about constant solutions leads to a perturbation series in the anharmonic terms of the potential. Not enough of the potential is probed to produce a leading term which contains the full classical result. Nonconstant solutions $x_{\rm cl}(\tau)$ are the analogs of instantons at finite temperature. For the double well (1.3), there are no such solutions for $\omega\beta\hbar<2\pi$.

In order to proceed with a semiclassical approximation we write (2.1) as

$$Z=\overline{N}\int_{-\infty}^{\infty}dx\int_{\substack{\text{all paths}\\ x(0)=x(\beta\hbar)=x}}Dx\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar}\left(d\tau\ \frac{\dot{x}^2}{2}+V\right)\right]. \tag{2.2}$$

Again $\overline{N}$ depends on the normalization of the measure. In (2.2) a new constraint has been introduced and integrated over. This constrained form of the partition function is what would have appeared naturally had a continuous basis been chosen to evaluate Z:

$$Z=\int_{-\infty}^{\infty}dx\,\langle x|e^{-\beta H}|x\rangle. \tag{2.3}$$

To evaluate (2.2) semiclassically, we shift by solutions to $\ddot{x}=V'$ whose end points are held fixed: $x(0)=x(\beta\hbar)=x$. Such solutions do exist at all temperatures.

We will show that the leading term in the loop expansion about such solutions gives the full $Z_{\rm cl}$

when $\hbar \to 0$.

First we discuss the pure quartic potential $H = p^2/2 + \lambda x^4$. The solutions to the classical equation $d^2x/d\tau^2 = 4\lambda x^3$ are

$$x_{\rm cl}(\tau) = \pm \frac{\bar\omega}{\sqrt{\lambda}\,\beta\hbar}\,\frac{1}{\operatorname{cn}\bar\omega(2\tau/\beta\hbar - 1)}, \tag{2.4}$$

where $\bar\omega$ is a function of x found by inverting (2.5):

$$x_{\rm cl}(0) = x_{\rm cl}(\beta\hbar) = x = \pm\frac{\bar\omega}{\sqrt{\lambda}\,\beta\hbar}\,\frac{1}{\operatorname{cn}\bar\omega}, \tag{2.5}$$

$$S_{\rm cl} \equiv \frac{1}{\hbar} I[x_{\rm cl}] = -\frac{\bar\omega^4}{\hbar^4 3\lambda\beta^3} + \frac{4\bar\omega^3}{\hbar^4 3\lambda\beta^3}\,\frac{\operatorname{sn}\bar\omega\operatorname{dn}\bar\omega}{\operatorname{cn}^3\bar\omega}, \tag{2.6}$$

$$\begin{aligned}\tilde N &\equiv \bar N\,\mathrm{Det}^{-1/2}\left(-\frac{\partial^2}{\partial\tau^2} + 12\lambda x_{\rm cl}{}^2\right)\\ &= \frac{\bar\omega^{1/2}}{\hbar(2\pi\beta)^{1/2}}\left[(\operatorname{cn}\bar\omega + \bar\omega\operatorname{sn}\bar\omega\operatorname{dn}\bar\omega)\left(\frac{\operatorname{sn}\bar\omega\operatorname{dn}\bar\omega}{\operatorname{cn}^4\bar\omega}\right)\right]^{-1/2}.\end{aligned} \tag{2.7}$$

The functions $\operatorname{cn}\bar\omega$, $\operatorname{sn}\bar\omega$, and $\operatorname{dn}\bar\omega$ are Jacobi elliptic functions all with modulus $k = 1/\sqrt{2}$. The functions $\operatorname{cn}\bar\omega$ and $\operatorname{sn}\bar\omega$ have quarter period $K(k)$, the complete elliptic integral of the first kind.[9] In the semiclassical approximation,

$$Z = \int_{-\infty}^{\infty} dx\, e^{-S_{\rm cl}}\tilde N \tag{2.8}$$

$$= \frac{2}{\hbar^2\beta^{3/2}(2\pi\lambda)^{1/2}}\int_0^{K(1/\sqrt{2})} d\bar\omega\; e^{-S_{\rm cl}}\left(\frac{\bar\omega\operatorname{cn}\bar\omega}{\operatorname{sn}\bar\omega\operatorname{dn}\bar\omega} + \bar\omega^2\right)^{1/2}, \tag{2.9}$$

where the change of variables (2.5) has been used to give (2.9). An asymptotic expansion for $\hbar \to 0$ can now be evaluated for (2.9) and we have

$$\begin{aligned}\lim_{\hbar\to 0} Z &= \lim_{\hbar\to 0}\frac{1}{\hbar\lambda^{1/4}\beta^{3/4}}\,\frac{1}{2(2\pi)^{1/2}}\,\Gamma(\tfrac14)[1 + O(\hbar^4\lambda\beta^3)]\\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\int_{-\infty}^{\infty} dx\, e^{-\beta(p^2/2 + \lambda x^4)}\\ &\equiv Z_{\rm cl}.\end{aligned} \tag{2.10}$$

We note that in this "massless" potential there is only one dimensionless parameter $\Lambda \equiv \hbar^4\lambda\beta^3$. The correct classical limit comes entirely from the semiclassical approximation (2.8) in spite of the fact that the integrand in (2.2) now has $\hbar$ appearing nontrivially in the action.

The calculations for the double-well potential are similar to those of the massless theory but more tedious. They will be summarized here briefly. The classical equation is $d^2x/d\tau^2 = -\omega^2 x + g^2x^3$. The solutions are as follows: for $|x| \leqslant \omega/g$,

$$x_{\rm cl}(\tau) = \pm\frac{\omega}{g}\left(\frac{2k^2}{1+k^2}\right)^{1/2}\operatorname{cd}_k\frac{\omega(\tau - \frac12\beta\hbar)}{(1+k^2)^{1/2}}, \tag{2.11}$$

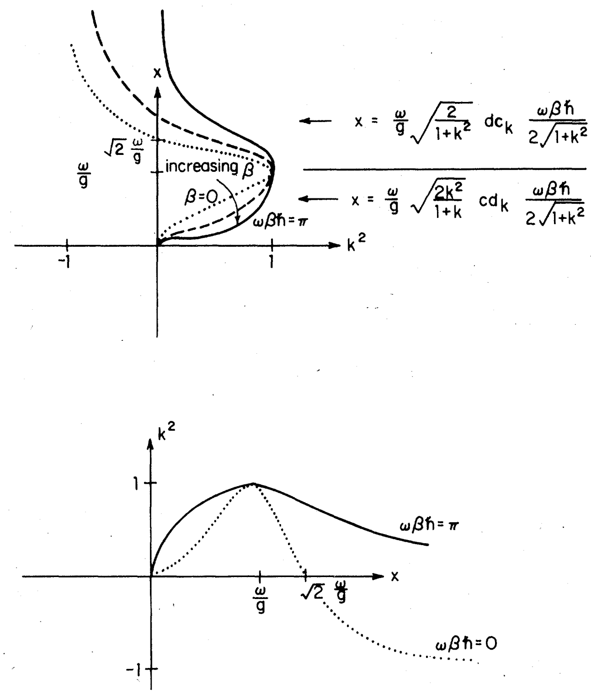

FIG. 1. Inversion of boundary conditions.

$$\begin{aligned}x_{\rm cl}(0) &= x_{\rm cl}(\beta\hbar) = x\\ &= \pm\frac{\omega}{g}\left(\frac{2k^2}{1+k^2}\right)^{1/2}\operatorname{cd}_k\frac{\omega\beta\hbar}{2(1+k^2)^{1/2}},\end{aligned} \tag{2.12}$$

where $0 \leqslant k^2 \leqslant 1$; for $|x| > \omega/g$,

$$x_{\rm cl}(\tau) = \pm\frac{\omega}{g}\left(\frac{2}{1+\mu^2}\right)^{1/2}\operatorname{dc}_\mu\frac{\omega(\tau - \frac12\beta\hbar)}{(1+\mu^2)^{1/2}}, \tag{2.13}$$

$$x = \pm\frac{\omega}{g}\left(\frac{2}{1+\mu^2}\right)^{1/2}\operatorname{dc}_\mu\frac{\omega\beta\hbar}{2(1+\mu^2)^{1/2}}, \tag{2.14}$$

where $-1 \leqslant \mu^2 \leqslant 1$.

For $\omega\beta\hbar < \pi$ Eqs. (2.12) and (2.14) have a unique inversion (k^2 or μ^2 is a single-valued function of x); see Fig. 1, for example. For $\omega\beta\hbar > \pi$ there exists more than one solution to $\ddot x = V'(x)$ with the

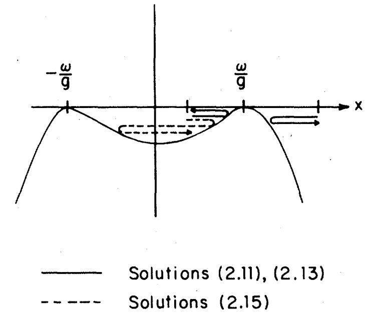

FIG. 2. Euclidean solutions.

boundary conditions $x(0)=x(\beta\hbar)=x$. Furthermore, for $\omega\beta\hbar\geq 2\pi n$, when x is such that $n4k(1+k^2)^{1/2}=\omega\beta\hbar$, where n is an integer greater than zero, there exists an additional set of solutions of the form

$$x(\tau)=\frac{x}{\bar{x}}\frac{\left\{\pm\left[\mathrm{sn}_k\frac{\omega\tau}{(1+k^2)^{1/2}}\right][(1-\bar{x}^2)(1-k^2\bar{x}^2)]^{1/2}+\bar{x}\,\mathrm{cn}_k\frac{\omega\tau}{(1+k^2)^{1/2}}\mathrm{dn}_k\frac{\omega\tau}{(1+k^2)^{1/2}}\right\}}{1-k^2\bar{x}^2\mathrm{sn}_k^2\frac{\omega\tau}{(1+k^2)^{1/2}}},$$

$$\bar{x}\equiv\frac{gx}{\omega}\left(\frac{1+k^2}{2k^2}\right)^{1/2}; \qquad (2.15)$$

see Fig. 2. In the zero-temperature limit $\beta\to\infty$, $k^2\to 1$, Eq. (2.15) becomes

$$x(\tau)=\frac{\omega}{g}\frac{\left[\pm\frac{1}{2}(\sinh\sqrt{2}\omega\tau)\left(1-\frac{g^2x^2}{\omega^2}+\frac{xg}{\omega}\right)\right]}{\cosh^2\frac{\omega\tau}{\sqrt{2}}-\frac{x^2g^2}{\omega^2}\sinh^2\frac{\omega\tau}{\sqrt{2}}}.$$

Note that $x_{\mathrm{cl}}(0)=x$ but

$$\lim_{\tau\to\infty}x_{\mathrm{cl}}(\tau)=\pm\,\omega/g.$$

These are the solutions which resemble the kink. When there are many solutions, the procedure is to add together their contributions.[4] Since we already have a low-temperature expression from WKB methods, in this paper we calculate for finite temperatures in the range $\omega\beta\hbar<\pi$. From Eq. (2.11),

$$S_{\mathrm{cl}}=\frac{\beta\omega^4}{4g^2}\left(\frac{1-k^2}{1+k^2}\right)^2+\frac{\omega^3}{\hbar g^2}\frac{4}{3}\frac{k^2-1}{(k^2+1)^{3/2}}\left\{\frac{k^2\,\mathrm{sn}_k\bar{\omega}\mathrm{cn}_k\bar{\omega}}{\mathrm{dn}_k^3\bar{\omega}}+\bar{\omega}+\left(\frac{k^2+1}{k^2-1}\right)\left[\frac{-k^2\mathrm{sn}_k\bar{\omega}\mathrm{cn}_k\bar{\omega}}{\mathrm{dn}_k\bar{\omega}}+E_k(\bar{\omega})\right]\right\},$$

$$\tilde{N}=\frac{1}{\hbar(2\pi\beta)^{1/2}}\,\bar{\omega}^{1/2}\frac{\mathrm{dn}_k^2\bar{\omega}}{\mathrm{sn}_k\bar{\omega}}[(k^2-1)\bar{\omega}+(k^2+1)E_k(\bar{\omega})+\mathrm{cn}_k\bar{\omega}\mathrm{ds}_k\bar{\omega}]^{-1/2}, \qquad (2.16)$$

where

$$\bar{\omega}\equiv\omega\beta\hbar/2(1+k^2)^{1/2}, \qquad (2.17)$$

and from (2.13),

$$S_{\mathrm{cl}}=\frac{\beta\omega^4}{4g}\left(\frac{1-\mu^2}{1+\mu^2}\right)^2+\frac{\omega^3}{\hbar g}\frac{4}{3}\frac{\mu^2-1}{(\mu^2+1)^{3/2}}\left\{-\frac{\mathrm{sn}_\mu\bar{\omega}\,\mathrm{dn}_\mu\bar{\omega}}{\mathrm{cn}^3{}_\mu\bar{\omega}}-\mu^2\bar{\omega}+\left(\frac{\mu^2+1}{\mu^2-1}\right)[-\mathrm{sn}_\mu\bar{\omega}\mathrm{dc}_\mu\bar{\omega}+E_\mu(\bar{\omega})-(1-\mu^2)\bar{\omega}]\right\}, \qquad (2.18)$$

$$\tilde{N}=\left\{2\pi\hbar\frac{2(1+\mu^2)^{1/2}}{\omega}\frac{\mathrm{sn}_\mu^2\bar{\omega}}{\mathrm{cn}_\mu^4\bar{\omega}}\left[\mathrm{cn}_\mu\bar{\omega}\,\mathrm{ds}_\mu\bar{\omega}+\frac{(\mu^2-1)\bar{\omega}}{\mu^2}+\frac{\mu^2+1}{\mu^2}E_\mu(\bar{\omega})\right]\right\}^{-1/2},$$

$$\bar{\omega}=\omega\beta\hbar/2(1+\mu^2)^{1/2}. \qquad (2.19)$$

To compute the partition function, let

$$Z=Z_A+Z_B,$$

$$Z_A=\int_{-\omega/g}^{\omega/g}dx\langle x|e^{-\beta H}|x\rangle, \qquad (2.20)$$

$$Z_B=\int_{-\infty}^{-\omega/g}dx\langle x|e^{-\beta H}|x\rangle+\int_{\omega/g}^{\infty}dx\langle x|e^{-\beta H}|x\rangle. \qquad (2.21)$$

In the semiclassical approximation,

$$Z_A=\frac{2}{\hbar(\pi\beta)^{1/2}}\frac{\omega}{g}\int_0^1 dk^2e^{-S_{\mathrm{cl}}}\left[\frac{\bar{\omega}^{1/2}[(k^2-1)\bar{\omega}+(k^2+1)E_k(\bar{\omega})+\mathrm{cn}_k\bar{\omega}\mathrm{dn}_k\bar{\omega}/\mathrm{sn}_k\bar{\omega}]^{1/2}}{2k(1+k^2)^{3/2}}\right]; \qquad (2.22)$$

with the change of variables (2.12), we have

$$\lim_{\hbar\to 0} Z_A = \frac{\omega}{g\hbar(\pi\beta)^{1/2}} \int_0^1 \frac{dk^2}{(1+k^2)^{3/2}} \exp\left[-\beta\frac{\omega^4}{4g^2}\left(\frac{1-k^2}{1-k^2}\right)^2\right]$$
$$= \frac{1}{\hbar(2\pi\beta)^{1/2}} \int_{-\omega/g}^{\omega/g} dz \exp\left[-\frac{\beta g^2}{4}\left(z^2-\frac{\omega^2}{g^2}\right)^2\right]$$
$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp \int_{-\omega/g}^{\omega/g} dz\, e^{-\beta[p^2/2+V(z)]}$$
$$= Z_A^{\mathrm{cl}}\,. \tag{2.23}$$

The change of variables $z=(\omega/g)\,[2k^2/(1+k^2)]^{1/2}$ has been used to derive (2.23). Similarly Eq. (2.21) in the semiclassical approximation is

$$Z_B = 2\int_{-1}^{1} d\mu^2\, e^{-S_{\mathrm{cl}}} \left[-\frac{1}{(2\pi\hbar)^{1/2}}\frac{\omega^{3/2}}{2g(1+\mu^2)^{7/4}}\right]$$
$$\times\left[\frac{(\mu^2-1)\bar{\omega}}{\mu^2}+\frac{(\mu^2+1)E_\mu(\bar{\omega})}{\mu^2}+\mathrm{ds}_\mu\bar{\omega}\,\mathrm{cn}_\mu\bar{\omega}\right]^{1/2},$$
$$\lim_{\hbar\to 0} Z_B = -\frac{\omega}{g}\frac{1}{\hbar(\pi\beta)^{1/2}}\int_{-1}^{1} d\mu^2 \exp\left[-\frac{\beta\omega^4}{4g^2}\left(\frac{1-\mu^2}{1+\mu^2}\right)^2\right]$$
$$\times\frac{1}{(1+\mu^2)^{3/2}}$$
$$= \frac{1}{\hbar(2\pi\beta)^{1/2}}\left(\int_{-\infty}^{-\omega/g} dz\, e^{-\beta V(z)} + \int_{+\omega/g}^{\infty} dz\, e^{-\beta V(z)}\right). \tag{2.24}$$

The change of variables is $z=(\omega/g)\,[2/(1+\mu^2)]^{1/2}$ to derive (2.24).

III. EUCLIDEAN CORRELATION FUNCTION

We now calculate the imaginary-time correlation function using the method of Sec. II which gave an expansion for Z containing Z_{cl} in the first term. The Euclidean path-integral representation for the correlation function is

$$\mathcal{C}\left(\frac{\tau}{\hbar}\right) = \frac{\bar{N}}{Z}\int_{-\infty}^{\infty} dx \int Dx\, x(\tau)x(0)\exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} dt[\dot{x}^2/2+V(x)]\right\}. \tag{3.1}$$

We find that in terms of the variable $\sigma\equiv\tau/\hbar$ the loops in this expansion of $\mathcal{C}(\sigma)$ are higher order in $\hbar$. With the restriction $0\leq\tau\leq\beta\hbar$, it is hard to see how to extract the information from $\mathcal{C}(\sigma)$ which was available from the $\sigma\to\infty$ limit at zero temperature. When the analytic continuation[5] of this expansion is made,

$$\sigma\to it/\hbar,\quad C(t)=\mathcal{C}(it/\hbar),$$

the loops are no longer higher order in $\hbar$. This is described below for the pure quartic potential $V=\lambda x^4$ in order to illustrate how the approximation breaks down. It is an unexpected feature in the analysis of the semiclassical estimates of imaginary-time correlation functions.

The Euclidean correlation function is

$$\mathcal{C}\left(\frac{\tau}{\hbar}\right) = \frac{1}{Z}\bar{N}\int_{\infty}^{\infty} dx \int_{\substack{\text{all paths}\\ x(0)=x(\beta\hbar)=x}} Dx\, x(\tau)x(0)\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau(\tfrac{1}{2}\dot{x}^2+\lambda x^4)\right]. \tag{3.2}$$

After shifting by $x_{\mathrm{cl}}(\tau)$ [see (2.4) and (2.5)], we obtain

$$\mathcal{C}\left(\frac{\tau}{\hbar}\right) = \frac{\bar{N}}{Z}\int_{-\infty}^{\infty} dx\, x\, e^{-S_{\mathrm{cl}}}\int Dy \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left[y\left(\frac{-d^2}{2d\tau^2}+6\lambda x_{\mathrm{cl}}^2\right)y+W(x_{\mathrm{cl}},y)\right]\right\}[x_{\mathrm{cl}}(\tau)+y(\tau)]. \tag{3.3}$$

We now perturb in

$$W(x_{\mathrm{cl}},y)=4\lambda x_{\mathrm{cl}}y^3+\lambda y^4. \tag{3.4}$$

What we call the semiclassical approximation $\mathcal{C}_0(\tau/\hbar)$ to $\mathcal{C}(\tau/\hbar)$ is

$$\mathcal{C}_0\left(\frac{\tau}{\hbar}\right) = \frac{1}{Z}\int_{-\infty}^{\infty} dx\, x\, x_{\mathrm{cl}}(\tau)\tilde{N}e^{-S_{\mathrm{cl}}}, \tag{3.5}$$

where $\tilde{N}$ and S_{cl} are given by (2.6) and (2.7). In terms of σ, (3.5) becomes

$$\mathcal{C}_0(\sigma) = \frac{1}{Z}\int_{-\infty}^{\infty} dx\, x\, x_{\mathrm{cl}}(\hbar\sigma)\tilde{N}e^{-S_{\mathrm{cl}}}. \tag{3.6}$$

The $\hbar\to 0$ limit of (3.6) is independent of σ and cannot be analytically continued to give the small-$\hbar$ limit of $C(t)$. If we continue $\tau\to it$ in (3.5) and let $\hbar\to 0$,

$$\lim_{\hbar\to 0} C_0(t) = \frac{4}{\Gamma(\frac{1}{4})(\lambda\beta)^{1/2}}\int_0^{\infty} dy\, e^{-y^4}y^2\,\mathrm{cn}\left[2\left(\frac{\lambda}{\beta}\right)^{1/4} yt\right]. \tag{3.7}$$

The classical correlation function is defined by

$$C_{\mathrm{cl}}(t) = \frac{1}{Z_{\mathrm{cl}}}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\int_{-\infty}^{\infty} dx\, e^{-\beta[p^2/2+V(x)]}\bar{x}(t)\bar{x}(0), \tag{3.8}$$

where $\bar{x}(t)$ is a solution to the real-time equation $\ddot{\bar{x}}=-V'(\bar{x})$ with boundary conditions $\bar{x}(0)=x$ and $\dot{\bar{x}}(0)=p$. For $V=\lambda x^4$,

$$C_{\rm cl}(t)=\frac{1}{\Gamma(\frac{1}{4})(\lambda\beta)^{1/2}}\,8\left(\frac{2}{\pi}\right)^{1/2}\times\int_0^\infty dy\,e^{-y^4}y^4\{K{\rm cn}\gamma y+2{\rm ds}\gamma y[\gamma yE-KE(\gamma y)]\}\,, \tag{3.9}$$

where $\gamma\equiv 2(\lambda/\beta)^{1/4}t$, a dimensionless time variable, and the elliptic integrals and functions in (3.7), (3.9), and (3.11) have modulus $k=1/\sqrt{2}$. Clearly (3.7) is not equal to (3.9). We now evaluate the one-loop[10] tadpole contribution $\mathcal{C}_1(\tau/h)$ to (3.2) as follows:

$$\mathcal{C}_1\left(\frac{\tau}{\hbar}\right)\equiv\frac{1}{Z}\bar{N}\int_{-\infty}^{\infty}dx\,xe^{-S_{\rm cl}}\left(\frac{-4\lambda}{\hbar}\right)\int_0^{\beta\hbar}d\tau'x_{\rm cl}(\tau')\int Dy\,y(\tau)y^3(\tau')\exp\left[-\frac{1}{2\hbar}\int_0^{\beta\hbar}d\tau''y\left(\frac{-d^2}{d\tau''^2}+12\lambda x_{\rm cl}{}^2\right)y\right]. \tag{3.10}$$

Continuing (3.10) to real time and letting $\hbar\to 0$, we find a nonzero answer:

$$\lim_{\hbar\to 0}C_1(t)=\frac{1}{\Gamma(\frac{1}{4})(\lambda\beta)^{1/2}}\,\frac{1}{2}\int_0^\infty dy\,e^{-y^4}\times\left(\frac{{\rm cn}\gamma y\,{\rm sn}^2\gamma y}{y^2}+\frac{1}{y}\frac{\partial}{\partial y}{\rm cn}\gamma y\right). \tag{3.11}$$

Equation (3.11) combined with (3.7), however, still does not reproduce the classical Boltzmann expression (3.9). We have studied the contributions of the two-loop corrections as well.

The results can be summarized:

$$\lim_{\hbar\to 0}\mathcal{C}_i(\sigma)\big|_{{\rm fixed}\,\sigma}\sim(h\sigma)^{4i}\quad\text{for } i=0,1,2\,. \tag{3.12}$$

Thus we see why a semiclassical expansion of $\mathcal{C}(\sigma)$ cannot be used to obtain a semiclassical expansion of $C(t)$.

To circumvent this problem and still make use of semiclassical methods, we introduce a path-integral representation for the real-time correlation function directly.

IV. REAL-TIME PATH-INTEGRAL REPRESENTATION

The real-time correlation function is defined to be

$$C(t)=\frac{1}{Z}{\rm Tr}e^{-\beta H}x(t)x(0)=\frac{1}{Z}\int_{-\infty}^{\infty}dx\langle x|e^{-\beta H}e^{iHt/\hbar}x(0)e^{-iHt/\hbar}x(0)|x\rangle\,. \tag{4.1}$$

As it stands, (4.1) has an awkward path-integral representation. An attempt to find a simpler expression by the continuation $t\to -i\hbar\sigma$ or $\beta\to iB/\hbar$ leads to the difficulties of Sec. III. Making use of completeness, we write (4.1) as

$$C(t)=\frac{1}{Z2\pi\hbar}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dp\,F_1(x,p)F_2(x,p,t)\,, \tag{4.2}$$

where

$$F_1(x,p)\equiv\int_{-\infty}^{\infty}dx_1\langle x|e^{-\beta H}|x_1\rangle e^{ip(x-x_1)/\hbar} \tag{4.3}$$

and

$$F_2(x,p,t)\equiv\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dx_2\,e^{ip(x_2-x)/\hbar}\langle x_2|e^{iHT/\hbar}|y\rangle\times\langle y|e^{-iHT/\hbar}x(t)x(0)|x\rangle\,, \tag{4.4}$$

where the dummy time T with $0<t<T$ has been introduced. The two matrix elements in (4.4) can be represented as real-time path integrals in the standard way and their semiclassical approximations are well known.[11]

As long as t, T are held fixed it is straightforward to evaluate the two integrals in (4.4) by the stationary-phase method. The result is

$$\lim_{\hbar\to 0}F_2(t;x,p)=\bar{x}(t;x,p)x\,.$$

The function $\bar{x}(t;x,p)$ solves $\ddot{x}=-V'(x)$ with $\bar{x}(0;x,p)=x$ and $\dot{\bar{x}}(0;x,p)=p$.

We will now show by direct calculation for the double well (1.3) that

$$\lim_{\hbar\to 0}F_1(x,p)=e^{-\beta(p^2/2+V)}\,.$$

In the semiclassical approximation,

$$\langle x|e^{-\beta H}|x_1\rangle=\tilde{N}_\beta(x_1,x)e^{-S_{\rm cl}(x_1,x)}\,. \tag{4.5}$$

In the double well, for $|x|\leq\omega/g$ and $|x_1|\leq\omega/g$,

$$S_{\rm cl}(x_1,x)=\beta V(x)+\frac{\beta\omega^4}{g^2}\left(\frac{1-k^2}{1+k^2}\right)^2\left[\frac{1}{{\rm dn}_k{}^2\omega_1}-\frac{1}{{\rm dn}_k{}^4\omega_1}+\frac{2}{\bar{\omega}}\int_{\omega_1}^{\omega_1+\bar{\omega}}dy\times\left(\frac{1}{{\rm dn}_k{}^4y}-\frac{1}{{\rm dn}_k{}^2y}\right)\right], \tag{4.6}$$

$$\tilde{N}_\beta(x_1,x)=\left\{2\pi\hbar\left(\frac{-(1+k^2)^{1/2}}{\omega}\right)u_1(K-\omega_1)\times u_1(K-\omega_1-\bar{\omega})[u_2(K-\omega_1-\bar{\omega})-\bar{u}_2(K-\omega_1)]\right\}^{-1/2}, \tag{4.7}$$

where

$$x_1=\pm\frac{\omega}{g}\left(\frac{2k^2}{1+k^2}\right)^{1/2}{\rm cd}_k(\bar{\omega}+\omega_1)\,,$$

$$x=\pm\frac{\omega}{g}\left(\frac{2k^2}{1+k^2}\right)^{1/2}\mathrm{cd}_k\omega_1\,, \tag{4.8}$$

$$\bar{\omega}\equiv\frac{\omega\beta h}{(1+k^2)^{1/2}}\,,$$

$$u_1(r)=\mathrm{cn}_k r\,\mathrm{dn}_k r\,, \tag{4.9}$$

$$\bar{u}_2(r)=\int_0^r\frac{dr'}{u_1^2(r')}\,.$$

For $|x|>\omega/g$, $|x_1|>\omega/g$,

$$S_{c1}=\beta V(x)+\frac{\omega^4\beta}{g^2}\left(\frac{1-k^2}{1+k^2}\right)^2$$

$$\times\left[\frac{1}{\mathrm{cn}_k^2\omega_1}-\frac{1}{\mathrm{cn}_k^4\omega_1}+\frac{2}{\bar{\omega}}\int_{\omega_1}^{\omega_1+\bar{\omega}}dy\left(\frac{1}{\mathrm{cn}_k^4 y}-\frac{1}{\mathrm{cn}_k^2 y}\right)\right], \tag{4.10}$$

where

$$x_1=\pm\frac{\omega}{g}\left(\frac{2}{1+k^2}\right)^{1/2}\mathrm{dc}_k(\omega_1+\bar{\omega})\,,$$

$$x=\pm\frac{\omega}{g}\left(\frac{2}{1+k^2}\right)^{1/2}\mathrm{dc}_k\omega_1\,, \tag{4.11}$$

and $\tilde{N}_\beta(x_1,x)$ is given by (4.7) with (4.11) replacing (4.8) and (4.12) replacing (4.9):

$$u_1(r)=\frac{\mathrm{cn}_k r\,\mathrm{dn}_k r}{\mathrm{sn}^2 r}\,,$$

$$\bar{u}_2(r)=\int_0^r\frac{dr'}{u_1^2(r')}\,. \tag{4.12}$$

Therefore, using (4.5) as an approximation in (4.3), we find

$$\lim_{\hbar\to 0}F_1(x,p)$$

$$=e^{-\beta[p^2/2+V(x)]}\int_{-\infty}^{\infty}d\omega_1 e^{-(\beta/2)(\Gamma+ip)^2}\left(\frac{\beta}{2\pi}\right)^{1/2}\frac{d\Gamma}{d\omega_1}\,, \tag{4.13a}$$

where for $|x|\leq\omega/g$,

$$\Gamma=\frac{\omega^2}{g}(2k^2)^{1/2}\frac{k^2-1}{k^2+1}\,\frac{\mathrm{sn}_k\omega_1}{\mathrm{dn}_k^2\omega_1}\,, \tag{4.13b}$$

and for $|x|>\omega/g$,

$$\Gamma=\frac{\omega^2}{g}\sqrt{2}\,\frac{1-k^2}{1+k^2}\,\frac{\mathrm{sn}_k\omega_1}{\mathrm{cn}_k^2\omega_1}\,. \tag{4.13c}$$

Then with the final change of variables $\omega_1\to\Gamma+ip$, Eq. (4.13a) becomes

$$\lim_{\hbar\to 0}F_1(x,p)=e^{-\beta[p^2/2+V(x)]}\,. \tag{4.14}$$

We have outlined an expansion for $C(t)$ which gives

$$\lim_{\hbar\to 0}C(t)=C_{c1}(t)\,, \tag{4.15}$$

which is correct at fixed t. The stationary-phase evaluation of (4.4) is, however, inadequate when T and t are becoming arbitrarily large as $\hbar\to 0$:

$$\lim_{\hbar\to 0}\lim_{t\to\infty}F_2\neq\lim_{t\to\infty}\lim_{\hbar\to 0}F_2\,. \tag{4.16}$$

Thus (4.15) is not valid in this asymptotic region of t. In fact, $C(t)$ is an almost periodic function[12] and its $t\to\infty$ limit does not exist. This matter is discussed in the Appendix.

V. CLASSICAL CORRELATION FUNCTION

In Sec. IV, it is shown that at fixed time t

$$C(t)=C_{c1}(t)+(\text{terms of higher order in }\hbar)\,. \tag{5.1}$$

Thus we study $C_{c1}(t)$ as a first approximation to $C(t)$.

The classical correlation function $C_{c1}(t)$ for

$$V=\frac{g^4}{4}\left(x^2-\frac{\omega^2}{g^2}\right)^2$$

is again given by (3.8) and

$$\bar{x}(t)=\frac{\omega}{g}\,\frac{\sqrt{2}}{(2-k^2)^{1/2}}\mathrm{dn}_k\frac{\omega(t-t_0)}{(2-k^2)^{1/2}}\,, \tag{5.2}$$

$$\bar{x}(0)\equiv x=\frac{\omega\sqrt{2}}{g(2-k^2)^{1/2}}\mathrm{dn}_k\frac{\omega t_0}{(2-k^2)^{1/2}}\,, \tag{5.3}$$

$$\dot{\bar{x}}(0)\equiv p=\frac{k^2\omega^2}{g}\,\frac{\sqrt{2}}{2-k^2}\,\mathrm{sn}\frac{\omega t_0}{(2-k^2)^{1/2}}\mathrm{cn}_k\frac{\omega t_0}{(2-k^2)^{1/2}}\,, \tag{5.4}$$

with the change of variables

$$\omega t_0/(2-k^2)^{1/2}\equiv\phi \text{ and } \omega/(2-k^2)^{1/2}\equiv w: \tag{5.5}$$

$$C_{c1}(t)=\frac{1}{Z_{c1}2\pi h}\int_{\omega/\sqrt{2}}^{\infty}dw\int_{-2k}^{2k}d\phi\,\frac{4w^2}{g^4}(2w^2-\omega^2)\exp\left[-\frac{\beta}{4g^2}(2w^2-\omega^2)^2\right]\mathrm{dn}_k\phi\,\mathrm{dn}_k(wt-\phi)\,. \tag{5.6}$$

Equation (5.6) is a complicated function of wt and $\beta\omega^4/g^2$ and we estimate it for large wt:

$$\lim_{t\to\infty}C_{c1}(t)=\sqrt{\beta}\,\frac{\omega^4}{g^3}\,\frac{\int_0^1\frac{dk^2}{K(k^2)}\frac{k^2(2\pi)^{3/2}}{(2-k^2)^{7/2}}\exp\left[\frac{-\beta\omega^4}{4g^2}\left(\frac{k^2}{2-k^2}\right)^2\right]}{\int_0^1 dy\exp\left[\frac{-\beta\omega^4}{4g^2}(y^2-1)^2\right]}\,. \tag{5.7}$$

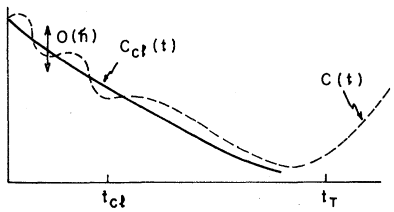

FIG. 3. The classical correlation function $C_{cl}(t)$ and the quantum correlation function $C(t)$.

The two integrals in (5.7) are each functions of the dimensionless constant $\beta\omega^4/g^2$. For high temperatures, the denominator behaves like $(\beta\omega^4/g^2)^{-1/4}$ and the numerator goes to a constant. Equation (5.7) is thus a decreasing function of increasing temperature. Furthermore,

$$\lim_{\beta\to 0}\lim_{t\to\infty} C_{cl}(t)=0\,. \tag{5.8}$$

VI. DISCUSSION

The function $C(t)$ measures the correlation of position measurements at time zero and at time t. And in this way it gives an indication of the order in the system. The considerations of Sec. IV show that for moderately large times the system becomes disordered and the disorder increases with temperature as we expect.

The almost periodicity of $C(t)$ says that for very much larger times (these are times which go to infinity as $\hbar$ goes to zero) the position measurements are correlated. It is our speculation that the time at which this correlation reappears is very different for the single minimum potential and the double well when $\hbar$ is small.

Paths which contribute to this difference may be those real-time solutions which have an energy near that of the barrier height and therefore spend a large time near $x=0$. We do not study this very large t region in detail.

The limit of $C(t)$ with t fixed as $\hbar\to 0$ has been given in Sec. IV. From that analysis we conclude that

$$\lim_{\hbar\to 0} C(t)=C_{cl}(t)+(\text{terms of higher order in }\hbar)\,. \tag{6.1}$$

That is to say, for moderately large times $C(t)$ is well approximated by $C_{cl}(t)$ to the extent that $\hbar$ is considered small. From Sec. V we know that $C_{cl}(t)$ is given by (5.7) at large t $[t>(\beta/\lambda)^{1/4}]$. Thus at moderately large times, $(\beta/\lambda)^{1/4}<t<t_T$, the quantum system is partially disordered by classical thermal fluctuations. This disordering is complete as $\beta\to 0$. The purely quantum tunneling transitions and associated instantons which are the only contributors to disorder at zero temperature are absent in the fixed-t, $\hbar\to 0$ approximation.

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APPENDIX

A function $f(t)$ is almost periodic if for each $\epsilon>0$ there exists $T(\epsilon)>0$ with the property that any interval of length $T(\epsilon)$ contains at least one point τ such that

$$|f(t+\tau)-f(t)|<\epsilon \tag{A1}$$

for all t.

A periodic function is almost periodic, and it is a theorem that a uniformly convergent series of almost periodic functions is almost periodic.

We will show that for a potential which rises at least as x^2 for $|x|\to\infty$, $C(t)$ is almost periodic. In a basis diagonalizing H,

$$C(t)=\frac{1}{Z}\sum_{m=0} e^{-\beta E_m}\langle m|x(t)x(0)|m\rangle\,. \tag{A2}$$

Now

$$\langle m|x(t)x(0)|m\rangle=\sum_n |\langle m|x|m\rangle|^2\, e^{i(E_m-E_n)t/\hbar} \tag{A3}$$

and is almost periodic if the sum converges uniformly. Since each term is bounded by its value at $t=0$ and since the sum

$$\sum_n |\langle m|x|n\rangle|^2=\langle m|x^2|m\rangle<\infty \tag{A4}$$

converges, we can conclude from the "M test" that (A3) converges uniformly.

Thus, (A2) is a sum of almost periodic functions. Again each term is bounded by its value at $t=0$ and we must consider

$$\sum_m e^{-\beta E_m}\langle m|x^2|m\rangle\,. \tag{A5}$$

For the potentials under consideration, although $\langle m|x^2|m\rangle$ may grow as a power of m, E_m will also,[13] and (A5) will converge. From another application of the M test we conclude that (A2) converges uniformly and that $C(t)$ is almost periodic.

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[8]Under an arbitrary small variation $x(t)\to x+\Delta x$, the action

$$I[x]\equiv\int_0^{\beta\hbar}dt[\tfrac{1}{2}\dot{x}^2+V(x)]\to I+\delta I+\dot{x}(t)\Delta x(t)\bigg|_0^{\beta\hbar}.$$

where

$$\delta I=\tfrac{1}{2}\int_0^{\beta\hbar}dt\Delta x\left(\frac{-d^2}{dt^2}+V''(x)\right)\Delta x$$

Since we vary on a space of periodic paths, $\Delta x(0)=\Delta x(\beta\hbar)$. The surface term in δI is then given by $[\dot{x}(\beta\hbar)-\dot{x}(0)]\,\Delta x(0)$. Thus for a true minimum ($\delta I=0$ for arbitrary periodic Δx), $\dot{x}(\beta\hbar)=\dot{x}(0)$.

[9]Our notation follows P. F. Byrd and M. D. Friedman, *Handbook of Elliptic Integrals for Engineers and Scientists* (Springer, New York, 1971).

[10]The loop expansion is normally equivalent to an expansion in powers of $\hbar$. What we show here is that for these finite-temperature semiclassical calculations this is not so. Rather, each loop is a complicated function of $\hbar$.

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