Semiclassical approximation to the partition function of a particle in D dimensions

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We use a path integral formalism to derive a semiclassical series for the partition function of a particle in D dimensions. In particular we analyze the case of attractive central potentials, obtaining explicit expressions for the fluctuation determinant and for the semiclassical two-point function in the special cases of the harmonic and single-well quartic anharmonic oscillators. The specific heat of the latter is compared to precise WKB estimates. We conclude by discussing the possible extension of our results to field theories.

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I. INTRODUCTION

As is well known [1–4], the partition function of a particle of mass m interacting with a potential $V(\mathbf{x})$ and a thermal reservoir at temperature T can be written as a path integral ($\beta=1/k_BT$):

$$Z(\beta)=\int_{\mathbb{R}^D} d^D\mathbf{x}_0\,\rho(\beta;\mathbf{x}_0,\mathbf{x}_0), \tag{1a}$$

$$\rho(\beta;\mathbf{x}_0,\mathbf{x}_0)=\int_{\mathbf{x}(0)=\mathbf{x}_0}^{\mathbf{x}(\beta\hbar)=\mathbf{x}_0}[\mathcal{D}\mathbf{x}(\tau)]\,e^{-S[\mathbf{x}]/\hbar}, \tag{1b}$$

$$S[\mathbf{x}]=\int_0^{\beta\hbar}d\tau\left[\frac{1}{2}m\left(\frac{d\mathbf{x}}{d\tau}\right)^2+V(\mathbf{x})\right]. \tag{1c}$$

This path integral may be approximated in a number of ways: depending on the circumstances, one may resort to perturbation theory around exactly soluble harmonic oscillator calculations, variational estimates, or lattice Monte Carlo calculations (such techniques carry over to quantum statistical field theory, where free fields play the role of unperturbed uncoupled harmonic oscillators). Semiclassical techniques can also be used in approximating this integral. It is their virtues and shortcomings in applications to statistical mechanics that we intend to discuss.

Semiclassical techniques have proven extremely important in a discussion of the transition from quantum to classical mechanics [5,6]. In the present context, however, we shall use them in the opposite sense: to systematically incorporate fluctuations (thermal and quantum) into a description that has one or more solutions of the ''Euclidean'' equations of motion as its starting point. (Heretofore, we call these solutions ''trajectories'' or ''classical paths.'') The Euclidean character is of crucial importance: first, it restricts the trajectories to be global minima of the Euclidean action [7]—any others are exponentially suppressed; in addition, it leads to classical mechanics problems whose potential is *minus* the physical one. Since we are interested in traces of operators, only closed trajectories will contribute. All this dramatically reduces the number of trajectories. In specific examples of harmonic and single-well quartic anharmonic oscillators, only one trajectory exists once the initial position and ''time of flight'' $\beta\hbar$ are fixed.

Thanks to the features described in the previous paragraph, in a recent paper [8] we were able to construct a full semiclassical series for the partition function of a particle in one dimension from the mere knowledge of the trajectories. We obtained fluctuation determinants in a straightforward manner, bypassing the solution of the equivalent boundary-value problems, generated all the terms of the series in a systematic way, and showed that each term has a nonperturbative character, corresponding to sums over infinite subsets of perturbative graphs. Furthermore, we showed [9] that the construction actually contains *all* the perturbative diagrams and many more. As an application of the method, we evaluated the ground-state energy and the specific heat of the single-well quartic anharmonic oscillator, for the former achieving good agreement with precise numerical results [10], and for the latter a result which has the correct high temperature limit, in contrast with the one obtained via conventional perturbation theory around the minima of the potential.

In this paper, we present a D-dimensional generalization of the method. Indeed, we are able to prove, as in the one-

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dimensional case, that it is possible to evaluate each term of the semiclassical series for the partition function using the classical path(s) as the only input. For the sake of simplicity, we concentrate on the case of attractive central potentials. In such potentials, as will be shown below, the only trajectories that contribute to the partition function are the ones with zero angular momentum. The discussion of arbitrary potentials is left for the Appendix. As examples, we consider the isotropic harmonic oscillator and the single-well quartic anharmonic oscillator; in particular, we compute the specific heat of the latter in the lowest order semiclassical approximation for a few values of the temperature and for $D=1,2$, and 3.

The paper is organized as follows: Section II presents the derivation of the semiclassical series for a generic potential in an arbitrary number of dimensions, and explicit formulas for the fluctuation determinant and the semiclassical two-point function in the particular case of attractive central potentials. Section III illustrates these results in the cases of harmonic oscillators and single-well quartic anharmonic oscillators. Section IV presents our conclusions. In the Appendix, we show how to obtain the fluctuation determinant and the semiclassical two-point function in the case of an arbitrary potential in D dimensions.

II. SEMICLASSICAL EXPANSION IN STATISTICAL MECHANICS

A. General formalism

The procedure to generate a semiclassical series for $Z(\beta)$ [Eq. (1) was carried out in detail in Ref. [8] for the one-dimensional case ($D=1$). Here we shall only sketch its generalization for arbitrary D (for a detailed discussion of the semiclassical expansion in quantum mechanics using path integrals, see Refs. [11,12]). The first step is to find the *minima* $\mathbf{x}_c(\tau)$ of the Euclidean action $S[\mathbf{x}]$. They satisfy the Euler-Lagrange equation

$$m\ddot{\mathbf{x}}_c-\nabla V(\mathbf{x}_c)=0, \tag{2}$$

subject to the boundary conditions $\mathbf{x}_c(0)=\mathbf{x}_c(\beta\hbar)=\mathbf{x}_0$; for simplicity, we shall assume here that there is only one minimum. The next step is to functionally expand the Euclidean action around it. Writing $\mathbf{x}(\tau)=\mathbf{x}_c(\tau)+\mathbf{u}(\tau)$, with $\mathbf{u}(0)=\mathbf{u}(\beta\hbar)=0$, we have $S[\mathbf{x}]=S[\mathbf{x}_c]+S_2[\mathbf{u}]+\delta S[\mathbf{u}]$, where

$$S_2[\mathbf{u}]\equiv\frac{1}{2}\int_0^{\beta\hbar}d\tau\, u_i(\tau)\left[-m\frac{d^2}{d\tau^2}\delta_{ij}+\partial_i\partial_j V(\mathbf{x}_c)\right]u_j(\tau), \tag{3a}$$

$$\delta S[\mathbf{u}]\equiv\int_0^{\beta\hbar}d\tau\,\delta V(\tau,\mathbf{u})$$
$$\equiv\int_0^{\beta\hbar}d\tau\sum_{n=3}^{\infty}\frac{1}{n!}\partial_{i_1}\cdots\partial_{i_n}V(\mathbf{x}_c)\,u_{i_1}(\tau)\cdots u_{i_n}(\tau); \tag{3b}$$

the indices $i,j,\ldots$ run from 1 to D, and repeated indices are summed. Inserting this decomposition of S into Eq. (1), and expanding $e^{-\delta S/\hbar}$ in a power series, yields the semiclassical expansion of $Z(\beta)$:

$$Z(\beta)=\int_{\mathbb{R}^D}d^D\mathbf{x}_0\,e^{-S[\mathbf{x}_c]/\hbar}\int_{\mathbf{u}(0)=0}^{\mathbf{u}(\beta\hbar)=0}[\mathcal{D}\mathbf{u}(\tau)]\times e^{-S_2[\mathbf{u}]/\hbar}\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{\delta S[\mathbf{u}]}{\hbar}\right)^n. \tag{4}$$

The first term of the series corresponds to the quadratic approximation to the partition function, which we denote by $Z_2(\beta)$:

$$Z_2(\beta)\equiv\int_{\mathbb{R}^D}d^D\mathbf{x}_0 e^{-S[\mathbf{x}_c]/\hbar}\int_{\mathbf{u}(0)=0}^{\mathbf{u}(\beta\hbar)=0}[\mathcal{D}\mathbf{u}(\tau)]e^{-S_2[\mathbf{u}]/\hbar}$$
$$=\int_{\mathbb{R}^D}d^D\mathbf{x}_0 e^{-S[\mathbf{x}_c]/\hbar}\Delta^{-1/2}, \tag{5}$$

where Δ is the determinant of the fluctuation operator $\mathcal{F}$:

$$\Delta=\det\mathcal{F},\quad \mathcal{F}_{ij}=-m\frac{d^2}{d\tau^2}\delta_{ij}+\partial_i\partial_j V(\mathbf{x}_c). \tag{6}$$

The other terms of series (4) lead to integrals of the type

$$\langle u_{i_1}(\tau_1)\ldots u_{i_k}(\tau_k)\rangle\equiv\int_{\mathbf{u}(0)=0}^{\mathbf{u}(\beta\hbar)=0}[\mathcal{D}\mathbf{u}(\tau)]\times e^{-S_2[\mathbf{u}]/\hbar}u_{i_1}(\tau_1)\cdots u_{i_k}(\tau_k). \tag{7}$$

Since the action $S_2[\mathbf{u}]$ is quadratic, one can show that

$$\langle u_{i_1}(\tau_1)\cdots u_{i_k}(\tau_k)\rangle=\hbar^{k/2}\Delta^{-1/2}\sum_P G_{i_{j_1}i_{j_2}}(\tau_{j_1},\tau_{j_2})\cdots G_{i_{j_{k-1}}i_{j_k}}(\tau_{j_{k-1}},\tau_{j_k}) \tag{8}$$

if k is even, and zero otherwise. Σ_P denotes the sum over all possible pairings of τ_{j_k}, and $G_{ij}(\tau,\tau')$ is the solution of

$$\left[-m\frac{d^2}{d\tau^2}\delta_{ij}+\partial_i\partial_j V(\mathbf{x}_c)\right]G_{jk}(\tau,\tau')=\delta_{ik}\,\delta(\tau-\tau'), \tag{9}$$

satisfying the boundary conditions

$$G_{jk}(0,\tau')=G_{jk}(\beta\hbar,\tau')=0. \tag{10}$$

In the Appendix we present a recipe for obtaining Δ and $G_{ij}(\tau,\tau')$ using the general solution of the equation of motion (2) as the only input.

B. Central potentials

To illustrate the formalism of Sec. II A, let us apply it to the case of central potentials, i.e., $V=V(r)$, where $r\equiv|\mathbf{x}|$. First of all, we note that, because of the radial symmetry, $\rho(\beta;\mathbf{x}_0,\mathbf{x}_0)$ can only depend on $r_0=|\mathbf{x}_0|$. Thus, without loss of generality, we may take $\mathbf{x}_0=r_0\,\mathbf{e}_1$, where $\mathbf{e}_1$ is the unit vector pointing in the x_1 direction, and perform the angular integration in Eq. (1a) to obtain

$$Z(\beta)=\frac{2\pi^{D/2}}{\Gamma(D/2)}\int_0^\infty dr_0\, r_0^{D-1}\,\rho(\beta;r_0\,\mathbf{e}_1;r_0\,\mathbf{e}_1). \qquad (11)$$

In general, there are many classical trajectories satisfying the boundary conditions $\mathbf{x}(0)=\mathbf{x}(\beta\hbar)=r_0\,\mathbf{e}_1$. However, they are all radial if the potential is purely attractive [i.e., $V'(r)>0$ for $r>0$]. Indeed, in this case the Euclidean motion is equivalent to that of a particle in a repulsive central potential, so that a closed classical trajectory necessarily has zero angular momentum. In addition, this trajectory is unique if the potential is smooth at the origin, i.e., $V'(0)=0$.

For a trajectory lying in the x_1 axis, $\mathbf{x}_c(\tau)=r_c(\tau)\,\mathbf{e}_1$, the fluctuation operator $\mathcal{F}$ is diagonal in the indices i and j. Indeed, since $V=V(r)$, we have

$$\partial_i\partial_j V(r)=\frac{V'(r)}{r}\,\delta_{ij}+\left[V''(r)-\frac{V'(r)}{r}\right]\frac{x_ix_j}{r^2}, \qquad (12)$$

which, for $x_i=r_c\,\delta_{i1}$, gives $\partial_1\partial_1V(r_c)=V''(r_c)$, $\partial_i\partial_iV(r_c)=r_c^{-1}\,V'(r_c)$ for $i=2,\ldots,D$, and $\partial_i\partial_jV(r_c)=0$ if $i\neq j$. Thus $\Delta=\Delta_l\Delta_t^{D-1}$, where

$$\Delta_l=\det[-m\,\partial_\tau^2+V''(r_c)],\quad \Delta_t=\det[-m\,\partial_\tau^2+r_c^{-1}\,V'(r_c)] \qquad (13)$$

(l and t stand for *longitudinal* and *transverse*, respectively).

The Green's function G_{ij} also becomes diagonal in this case: $G_{11}=G_l$, $G_{ii}=G_t$ for $i=2,\ldots,D$, and $G_{ij}=0$ if $i\neq j$, where

$$[-m\,\partial_\tau^2+V''(r_c)]\,G_l(\tau,\tau')=\delta(\tau-\tau'), \qquad (14a)$$

$$[-m\,\partial_\tau^2+r_c^{-1}\,V'(r_c)]\,G_t(\tau,\tau')=\delta(\tau-\tau'). \qquad (14b)$$

Δ_l and $G_l(\tau,\tau')$ are the fluctuation determinant and semiclassical Green's function that appear in the one-dimensional version of the problem, which was studied in detail in Ref. [8]. There, the following results were derived:

$$\Delta_l=\frac{2\pi\hbar}{m}\,\Omega_l(0,\beta\hbar),\quad G_l(\tau,\tau')=\frac{\Omega_l(0,\tau_<)\Omega_l(\tau_>,\beta\hbar)}{m\Omega_l(0,\beta\hbar)}, \qquad (15)$$

where $\tau_<(\tau_>)\equiv\min(\max)\{\tau,\tau'\}$, and

$$\Omega_l(\tau,\tau')\equiv\frac{\eta_a(\tau)\,\eta_b(\tau')-\eta_a(\tau')\,\eta_b(\tau)}{\eta_a(\tau')\,\dot\eta_b(\tau')-\dot\eta_a(\tau')\,\eta_b(\tau')}, \qquad (16)$$

with $\eta_a(\tau)$ and $\eta_b(\tau)$ any two linearly independent solutions of the homogeneus equation

$$[-m\,\partial_\tau^2+V''(r_c)]\,\eta(\tau)=0. \qquad (17)$$

By differentiating the equation of motion $m\ddot r_c-V'(r_c)=0$ with respect to τ, one can verify that $\eta_a(\tau)=\dot r_c(\tau)$ is one such solution. The other can be taken as [16] $\eta_b(\tau)=\dot r_c(\tau)\int_0^\tau d\tau'[\dot r_c(\tau')]^{-2}$. For such a choice, the denominator of $\Omega_l(\tau,\tau')$ is equal to 1 and, since $\eta_b(0)=0$, one has $\Delta_l=(2\pi\hbar/m)\,\eta_a(0)\,\eta_b(\beta\hbar)$. Because of these simplifying features, we shall refer to those solutions as the "canonical" solutions of Eq. (17).

In order to obtain Δ_t and $G_t(\tau,\tau')$ one simply replaces $\Omega_l(\tau,\tau')$ in Eq. (15) by

$$\Omega_t(\tau,\tau')\equiv\frac{\varphi_a(\tau)\,\varphi_b(\tau')-\varphi_a(\tau')\,\varphi_b(\tau)}{\varphi_a(\tau')\,\dot\varphi_b(\tau')-\dot\varphi_a(\tau')\,\varphi_b(\tau')}, \qquad (18)$$

where $\varphi_a(\tau)$ and $\varphi_b(\tau)$ are two linearly independent solutions of

$$[-m\,\partial_\tau^2+r_c^{-1}\,V'(r_c)]\,\varphi(\tau)=0. \qquad (19)$$

It immediately follows from the equation of motion that $\varphi_a(\tau)=r_c(\tau)$ is one such solution. Another one is $\varphi_b(\tau)=r_c(\tau)\int_0^\tau d\tau'[r_c(\tau')]^{-2}$. They form a pair of canonical solutions of Eq. (19).

III. APPLICATIONS

Using the results of Sec. II, we may write the quadratic approximation to the partition function as

$$Z_2(\beta)=\frac{2\pi^{D/2}}{\Gamma(D/2)}\int_0^\infty dr_0 r_0^{D-1}\,e^{-S[\mathbf{x}_c]/\hbar}(\Delta_l\Delta_t^{D-1})^{-1/2}. \qquad (20)$$

This can be readily calculated from a knowledge of $\mathbf{x}_c(\tau)$ alone. This will be acomplished below for both the harmonic and single-well quartic anharmonic oscillators.

A. Harmonic oscillator

As a first example, we consider the D-dimensional (isotropic) harmonic oscillator,

$$V(r)=\frac{1}{2}m\omega^2r^2. \qquad (21)$$

Since the potential is quadratic, $\delta V(\tau,\mathbf{u})=0$ and $Z(\beta)=Z_2(\beta)$. In addition, $r^{-1}\,V'(r)=V''(r)$, so that $\Delta_t=\Delta_l$. Thus

$$Z(\beta)=\frac{2\pi^{D/2}}{\Gamma(D/2)}\int_0^\infty dr_0\,r_0^{D-1}\,e^{-S[r_c]/\hbar}\,\Delta_l^{-D/2}. \qquad (22)$$

The solution of the equation of motion is straightforward, and yields

$$r_c(\tau)=\frac{r_0\cosh[\omega(\tau-\beta\hbar/2)]}{\cosh(\beta\hbar\omega/2)}. \qquad (23)$$

The classical action can be readily computed, giving

$$S[r_c]=m\omega r_0^2\tanh(\beta\hbar\omega/2). \qquad (24)$$

As solutions of Eq. (17) we may take $\eta_a(\tau)=\cosh(\omega\tau)$ and $\eta_b(\tau)=\sinh(\omega\tau)$. This gives $\Omega_l(\tau,\tau')=\omega^{-1}\sinh[\omega(\tau'-\tau)]$, so that

$$\Delta_l=\frac{2\pi\hbar\sinh(\beta\hbar\omega)}{m\omega}. \qquad (25)$$

Inserting Eqs. (24) and (25) into Eq. (22), and performing the integral, we obtain

$$Z(\beta)=[2\sinh(\beta\hbar\omega/2)]^{-D}, \tag{26}$$

which is the well-known result for the partition function of the D-dimensional harmonic oscillator.

B. Single-well quartic anharmonic oscillator

Let us now consider the potential

$$V(r)=\frac{1}{2}m\omega^2r^2+\frac{1}{4}\lambda r^4 \quad (\lambda>0). \tag{27}$$

In order to simplify the notation, it is convenient to replace r and τ by $q\equiv(\lambda/m\omega^2)^{1/2}r$ and $\theta\equiv\omega\tau$, respectively. In the new variables, the equation of motion reads

$$\frac{d^2q}{d\theta^2}=q+q^3, \tag{28}$$

whose solution, taking into account the boundary conditions, is

$$q_c(\theta)=q_t\mathrm{nc}(u_\theta,k), \tag{29}$$

where $\mathrm{nc}(u,k)\equiv 1/\mathrm{cn}(u,k)$ is one of the Jacobian elliptic functions [13–15], and

$$u_\theta=\sqrt{1+q_t^2}\left(\theta-\frac{\Theta}{2}\right),\quad k=\sqrt{\frac{2+q_t^2}{2(1+q_t^2)}}, \tag{30}$$

where $\Theta\equiv\beta\hbar\omega$. The relation between q_0 and q_t is obtained by taking $\theta=\Theta$ in Eq. (29):

$$q_0=q_c(\Theta)=q_t\mathrm{nc}u_\Theta\,. \tag{31}$$

(From now on we shall omit the k dependence in the Jacobian elliptic functions.)

The classical action can be written as $S[r_c]=(m^2\omega^3/\lambda)I[q_c]$, where

$$I[q]=\int_0^\Theta d\theta\left[\frac{1}{2}\dot{q}^2+U(q)\right],\quad U(q)=\frac{1}{2}q^2+\frac{1}{4}q^4. \tag{32}$$

Using $\frac{1}{2}\dot{q}_c^2-U(q_c)=-U(q_t)$, we may rewrite $I[q_c]$ as

$$I[q_c]=\Theta U(q_t)+2\int_{q_t}^{q_0}dq\sqrt{2[U(q)-U(q_t)]}. \tag{33}$$

Performing the integration and using Eq. (31) yields

$$I[q_c]=\Theta\left(\frac{1}{2}q_t^2+\frac{1}{4}q_t^4\right)+\frac{4}{3}\left\{-\sqrt{1+q_t^2}\left[\mathrm{E}(\varphi_\Theta,k)+\frac{1}{2}q_t^2u_\Theta\right]+\mathrm{sn}\,u_\Theta\left(1+\frac{1}{2}q_t^2\,\mathrm{nc}^2u_\Theta\right)\sqrt{1+\frac{1}{2}q_t^2(1+\mathrm{nc}^2u_\Theta)}\right\}, \tag{34}$$

where $\mathrm{E}(\varphi,k)$ denotes the elliptic integral of the second kind, and $\varphi_\theta\equiv\arccos[q_c(\theta)/q_0]=\arccos(\mathrm{cn}\,u_\theta)$.

The canonical solutions of Eqs. (17) and (19) are given by

$$\eta_a(\theta)=\omega q_t\sqrt{1+q_t^2}\frac{\mathrm{sn}\,u_\theta\,\mathrm{dn}\,u_\theta}{\mathrm{cn}^2u_\theta}, \tag{35a}$$

$$\eta_b(\theta)=\frac{1}{\omega^2q_t(1+q_t^2)}\frac{\mathrm{sn}\,u_\theta\,\mathrm{dn}\,u_\theta}{\mathrm{cn}^2u_\theta}\left[\frac{k^2-1}{k^2}u_\theta+\frac{1-2k^2}{k^2}\mathrm{E}(\varphi_\theta,k)-\frac{\mathrm{cn}\,u_\theta\,\mathrm{dn}\,u_\theta}{\mathrm{sn}\,u_\theta}+(k^2-1)\frac{\mathrm{sn}\,u_\theta\,\mathrm{cn}\,u_\theta}{\mathrm{dn}\,u_\theta}-(\theta\to 0)\right], \tag{35b}$$

$$\varphi_a(\theta)=q_t\,\mathrm{nc}\,u_\theta, \tag{35c}$$

$$\varphi_b(\theta)=\frac{\mathrm{nc}\,u_\theta}{\omega k^2q_t\sqrt{1+q_t^2}}[\mathrm{E}(\varphi_\theta,k)+(k^2-1)u_\theta-(\theta\to 0)]. \tag{35d}$$

Thus

$$\Delta_l=\frac{4\pi\hbar}{m\omega}\frac{\mathrm{sn}^2u_\Theta\,\mathrm{dn}^2u_\Theta}{\sqrt{1+q_t^2}\,\mathrm{cn}^4u_\Theta}\left[\frac{1-k^2}{k^2}u_\Theta+\frac{2k^2-1}{k^2}\mathrm{E}(\varphi_\Theta,k)+\frac{\mathrm{cn}\,u_\Theta\,\mathrm{dn}\,u_\Theta}{\mathrm{sn}\,u_\Theta}+(1-k^2)\frac{\mathrm{sn}\,u_\Theta\,\mathrm{cn}\,u_\Theta}{\mathrm{dn}\,u_\Theta}\right], \tag{36a}$$

$$\Delta_t=\frac{4\pi\hbar}{m\omega}\frac{\mathrm{nc}^2u_\Theta}{k^2\sqrt{1+q_t^2}}[\mathrm{E}(\varphi_\Theta,k)+(k^2-1)u_\Theta]. \tag{36b}$$

We now have all the necessary ingredients to compute the quadratic approximation to $Z(\beta)$,

$$Z_2(\beta)=\frac{2\pi^{D/2}}{\Gamma(D/2)}\left(\frac{m\omega^2}{\lambda}\right)^{D/2}\int_0^\infty dq_0\times q_0^{D-1}e^{-I[q_c]/g}(\Delta_l\Delta_t^{D-1})^{-1/2}, \tag{37}$$

where $g\equiv\hbar\lambda/m^2\omega^3$. However, to perform the integral over q_0 one must write $I[q_c]$, Δ_l, and Δ_t in terms of q_0. In view of Eq. (31), it is much simpler to change the variable of integration from q_0 to q_t,

$$Z_2(\beta)=\frac{2\pi^{D/2}}{\Gamma(D/2)}\left(\frac{m\omega^2}{\lambda}\right)^{D/2}\int_0^{q_\Theta}dq_t\left(\frac{\partial q_0}{\partial q_t}\right)_\Theta(q_t\,\mathrm{nc}\,u_\Theta)^{D-1}\times e^{-I[q_c]/g}(\Delta_l\Delta_t^{D-1})^{-1/2}, \tag{38}$$

where $q_\Theta=\lim_{q_0\to\infty}q_t(q_0,\Theta)$. The Jacobian $(\partial q_0/\partial q_t)_\Theta$ can be obtained directly from Eq. (31) by differentiation or, more simply, by using the identity [8]

$$\left(\frac{\partial q_0}{\partial q_t}\right)_\Theta=\frac{m\omega}{4\pi\hbar}\frac{U'(q_t)\Delta_l}{\sqrt{2[U(q_0)-U(q_t)]}}. \tag{39}$$

As an application, we may use Eq. (38) to calculate the specific heat of the D-dimensional single-well quartic anharmonic oscillator, given by

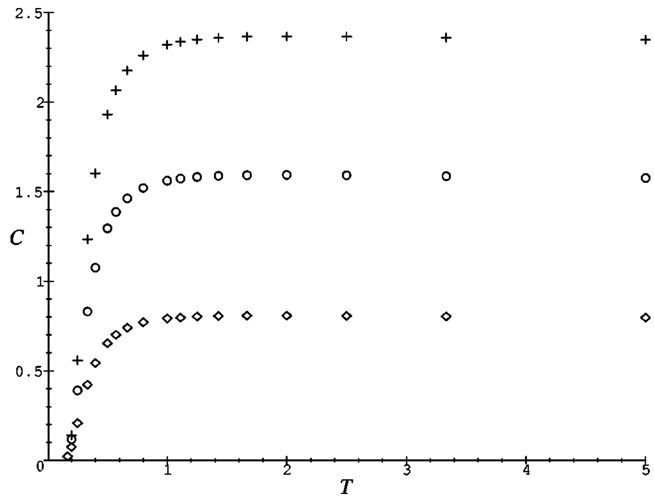

FIG. 1. Specific heat (in units of k_B) vs temperature ($T \equiv 1/\beta\hbar\omega$) for one- (diamonds), two- (circles), and three-dimensional (crosses) single-well quartic anharmonic oscillators in the semiclassical approximation. $g \equiv \hbar\lambda/m^2\omega^3 = 0.5$.

$$C = \beta^2 \frac{\partial^2}{\partial\beta^2} \ln Z. \tag{40}$$

Using the program MAPLE, we computed this expression for a few values of the temperature [17]. In Fig. 1, we present the results for $D=1$, 2, and 3. In Fig. 2, we compare the semiclassical approximation with (i) the classical result, in which the partition function is given by

$$Z_{\rm cl}(\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{D/2} \int d^D x e^{-\beta V(\mathbf{x})}; \tag{41}$$

(ii) with the lowest order WKB approximation, in which the energy levels entering the expression $Z = \Sigma_n e^{-\beta E_n}$ are given by the Bohr-Sommerfeld formula

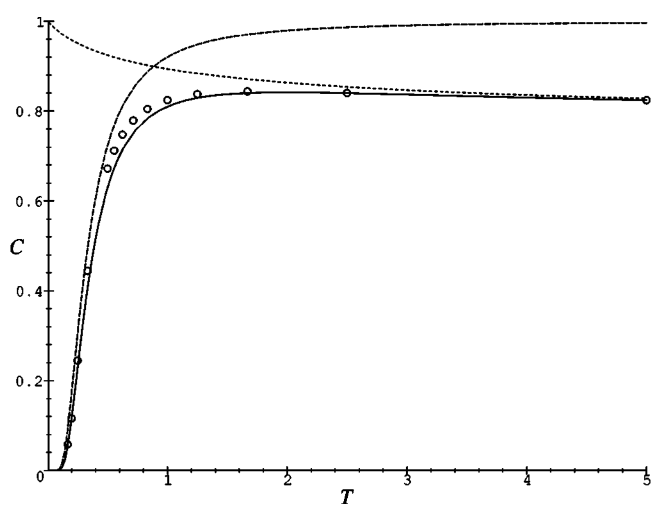

FIG. 2. Specific heat (in units of k_B) vs temperature ($T \equiv 1/\beta\hbar\omega$) for the one-dimensional harmonic oscillator (long-dashed line) and for the single-well quartic anharmonic oscillator: classical result (short-dashed line), semiclassical approximation (circles), and WKB approximation (solid line). $g \equiv \hbar\lambda/m^2\omega^3 = 0.2$.

$$\oint \sqrt{2m[E_n - V(x)]}\, dx = \left(n + \frac{1}{2}\right) h \quad (n = 0,1,2,\ldots); \tag{42}$$

and (iii) with the specific heat of the harmonic oscillator.

IV. CONCLUSIONS

The results of the previous sections confirm the findings of Refs. [8,9], and generalize them to arbitrary D. The semiclassical approach finds the minima of the Euclidean action and expands around them. As a result, it generates a series whose terms correspond to resummations of infinite numbers of perturbative graphs plus additional ones. Our calculations show that even the lowest order semiclassical estimates improve on perturbation theory at low temperatures and, in contrast to it, correctly describe the high temperature regime.

The comparison with WKB estimates, done for the one-dimensional case, is particularly interesting. Such estimates approximate the values of the energy levels of the single-well anharmonic oscillator to a high precision if $g \equiv \hbar\lambda/m^2\omega^3$ is small, even if we restrict ourselves to the lowest order WKB quantization condition, given by the Bohr-Sommerfeld formula [18]. They were then used to compute the partition function by actually performing the sums over eigenstates numerically. Thus the WKB results can be considered ''quasiexact.'' In contrast, the semiclassical approach directly approximates the *whole* sum. Its lowest order agrees well with the quasiexact WKB result at both high *and* low temperatures. At high T, this agreement just reflects the convergence of both results to the classical limit, something which is completely missed by perturbation theory. Only in the intermediate region does our result differ from the WKB result, although we expect this to be modified with the inclusion of next-to-leading orders. It is less accurate, as it approximates the whole sum, whereas the WKB result approximates each term in the sum; however, it does incorporate and improve upon the virtues of perturbation theory at low temperatures, and of the classical limit at high ones. Results for $D=2$ and $D=3$ do follow the same pattern, although we have not compared them to WKB estimates.

The advantage of this method is that it reduces the whole quantum problem to the computation of (a few) classical paths. From then on, a systematic procedure takes care of generating each term in the series. Paradoxically, this may also be its weakness: there are systems for which the action does not have a global minimum, but which are perfectly well defined quantum mechanically. The Coulomb potential is a good example; there, depending on the values of β and r_0, the number of classical paths may be two, one, or zero. In addition, only in the two-solution regime do we have minima. Even then, they are local, not global ones. Therefore, our starting point seems ill defined. This should not come as a surprise, however, since here the classical limit itself is ill defined, as the potential is unbounded below. As a matter of fact, even the usual time-slicing prescription to calculate the path integral must be modified in the case of the Coulomb potential [3]. Cases like this will require special consideration, although there exist suggestions in the literature as to how to treat similar situations of absence of classical paths in quantum mechanics [19]. Nevertheless, we expect the techniques presented here to be useful in any problem which can be reduced to the calculation of partition or correlation functions in equilibrium statistical mechanics, as long as it allows for a simple analysis of the minima of the Euclidean action.

Our next step is to investigate how the semiclassical treatment affects field-theoretic problems at finite temperature, where standard methods of computation of effective potentials rely on expansions around constant backgrounds. At finite temperature, these are not in general minima of the Euclidean action. This might lead to problems with the expansions around such backgrounds at high temperatures, of the same nature of those encountered by perturbation theory in quantum statistical mechanics. Even if we neglect any coordinate dependence of the fields, their dependence on Euclidean time is essential to satisfy equations of motion and boundary conditions that characterize classical paths. We expect this to have an effect on a variety of calculations.

Another problem of interest is to generalize our results to field theories with spherically symmetric classical solutions. An extension of the approach presented in this work to treat models containing nontrivial backgrounds (like instantons, monopoles, vortices, etc.) as classical solutions might lead to some new insights. Unfortunately, the extension of our results to field theories is not a straightforward process. In fact, we do not know how to construct a semiclassical propagator in general. The success of our program will depend on how well can we circumvent this difficulty.

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APPENDIX

Let $J(\tau,\tau')$ be the solution of the homogeneous differential equation

$$\left[-m\frac{d^2}{d\tau^2}\delta_{ij}+\partial_i\partial_j V(\mathbf{x}_c)\right]J_{jk}(\tau,\tau')=0, \tag{A1}$$

satisfying the initial conditions

$$J(\tau',\tau')=0, \quad \frac{\partial}{\partial\tau}J(\tau=\tau',\tau')=-\frac{1}{m}\mathbb{1}. \tag{A2}$$

This function is known as the Jacobi commutator [11,12]. It can be explicitly constructed as follows. Let $\mathbf{x}(\tau;\mathbf{a},\mathbf{b})$ be the solution of the equation of motion (2) satisfying the initial conditions $\mathbf{x}(0)=\mathbf{a}$, $\dot{\mathbf{x}}(0)=\mathbf{b}$. Let A and B be the $D\times D$ matrices defined as

$$A_{jk}(\tau)=\frac{\partial}{\partial a_k}x_j(\tau;\mathbf{a}=\mathbf{x}_0,\mathbf{b}=\mathbf{v}_0), \tag{A3}$$

$$B_{jk}(\tau)=\frac{\partial}{\partial b_k}x_j(\tau;\mathbf{a}=\mathbf{x}_0,\mathbf{b}=\mathbf{v}_0), \tag{A4}$$

where $\mathbf{v}_0=\dot{\mathbf{x}}_c(0)$. By differentiating Eq. (2) with respect to a_k and b_k (and taking $\mathbf{a}=\mathbf{x}_0$, $\mathbf{b}=\mathbf{v}_0$), one can show that they are solutions of Eq. (A1). They are also invertible for τ small enough [20] (but not zero). Indeed, $\mathbf{x}(\tau)=\mathbf{a}+\mathbf{b}\tau+O(\tau^2)$ when $\tau\to 0$; hence $A(\tau)=\mathbb{1}+O(\tau^2)$ and $B(\tau)=\tau\mathbb{1}+O(\tau^2)$. Therefore, the expression

$$J(\tau,\tau')=-\frac{1}{m}[A(\tau)A^{-1}(\tau')-B(\tau)B^{-1}(\tau')]\times[\dot{A}(\tau')A^{-1}(\tau')-\dot{B}(\tau')B^{-1}(\tau')]^{-1} \tag{A5}$$

makes sense, and one can easily verify that it satisfies Eqs. (A1) and (A2).

The Green's function $G(\tau,\tau')$ can be written in terms of the Jacobi commutator as

$$G(\tau,\tau')=J(\tau,0)M(0,\beta\hbar)J(\beta\hbar,\tau')\theta(\tau'-\tau)-J(\tau,\beta\hbar)M(\beta\hbar,0)J(0,\tau')\theta(\tau-\tau'), \tag{A6}$$

where $M(\tau,\tau')=-J(\tau',\tau)^{-1}$, and $\theta(\tau)$ is the Heaviside step function. To prove Eq. (A6) we need the following identities:

$$J(\tau,0)M(0,\beta\hbar)J(\beta\hbar,\tau')+J(\tau,\beta\hbar)M(\beta\hbar,0)J(0,\tau')=-J(\tau,\tau'), \tag{A7}$$

$$\partial_\tau J(\tau,0)M(0,\beta\hbar)J(\beta\hbar,\tau)+\partial_\tau J(\tau,\beta\hbar)M(\beta\hbar,0)J(0,\tau)=\frac{1}{m}\mathbb{1}. \tag{A8}$$

The first identity follows from the fact that both functions are solutions of the same second order differential equation [Eq. (A1)] and are equal at $\tau=0$ and $\tau=\beta\hbar$; the second follows from Eqs. (A2) and (A7).

Now, the proof of Eq. (A6): (i) it is a solution of Eq. (9) when $\tau<\tau'$ or $\tau>\tau'$; (ii) it satisfies the boundary conditions (10); (iii) it is continuous at $\tau=\tau'$,

$$G(\tau'+0,\tau')=G(\tau'-0,\tau') \tag{A9}$$

[use Eq. (A7) with $\tau=\tau'$], and (iv) its derivative with respect to τ has the discontinuity implied by Eq. (9),

$$\frac{\partial}{\partial\tau}G(\tau=\tau'+0,\tau')-\frac{\partial}{\partial\tau}G(\tau=\tau'-0,\tau')=-\frac{1}{m}\mathbb{1} \tag{A10}$$

[use Eq. (A8)].

Finally, the determinant Δ of the fluctuation operator $\mathcal{F}$ is given by

$$\Delta=(2\pi\hbar)^D\det[-J(\beta\hbar,0)]. \tag{A11}$$

This formula can be proven along the lines of Appendix 1 of Ref. [21].

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$$\eta_b(\tau)=\dot{r}_c(\tau)\left(C+\int_{\beta\hbar}^{\tau}\frac{d\tau'}{\dot{r}_c^2(\tau')}\right),$$

with C chosen in such a way that $\eta_b(\tau)$ and $\dot{\eta}_b(\tau)$ are continuous at $\tau=\beta\hbar/2$. See Ref. [8] for details.

[17] In order to compute the derivative in Eq. (40), we have approximated $\ln Z$ by a rational function using Thiele's interpolation formula. See *Handbook of Mathematical Functions* (Ref. [15]), formula 25.2.50.

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