Abstract

We use a path integral formalism to derive the semiclassical series for the partition function of a particle in $D$ dimensions. We analyze in particular 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 \(V(x)\) and a thermal reservoir at temperature \(T\) can be written as a path integral (\(\beta = 1/k_B T\)):

\[
Z(\beta) = \int d^D x_0 \rho(\beta; x_0, x_0),
\]

(1a)

\[
\rho(\beta; x_0, x_0) = \int_{x(0)=x_0}^{x(\beta h)=x_0} [Dx(\tau)] e^{-S[x]/\hbar},
\]

(1b)

\[
S[x] = \int_0^{\beta h} d\tau \left[ \frac{1}{2} m \left( \frac{dx}{d\tau} \right)^2 + V(x) \right].
\]

(1c)

This path integral may be approximated in a number of ways: depending on the circumstances, one may resort to perturbation theory around the exactly soluble harmonic oscillator, 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 the 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) to 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 \(-\) 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 the specific examples of the harmonic and single-well quartic anharmonic oscillators, only one trajectory exists once the initial position and “time-of-flight” \(\beta h\) are fixed.

Thanks to the features described in the previous paragraph, in a recent paper \[8\] we were able to construct the 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, by-passing the solution of the equivalent boundary-value problems, generated all the terms of the series in a systematic way, and could show that each term has a non-perturbative 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, achieving for the former 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
taken via conventional perturbation theory around the minima of the potential.

In this article, we present the $D$-dimensional generalization of the method. Indeed, we
are able to prove, as in the one-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 for arbitrary potentials
is left for an 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 article is organized as follows: Section II presents the derivation of the semiclassical
series for a generic potential in an arbitrary number of dimensions, and the explicit formulae
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 the
harmonic 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. THE 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 $x_c(\tau)$ of the Euclidean action $S[x]$. They satisfy the Euler-Lagrange equation

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

subject to the boundary conditions $x_c(0) = x_c(\beta \hbar) = x_0$; 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 $x(\tau) = x_c(\tau) + u(\tau)$, with $u(0) = u(\beta \hbar) = 0$, we have $S[x] =
S[x_c] + S_2[u] + \delta S[u]$, where

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

(3a)

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

(3b)

the indices $i, j, \ldots$ run from 1 to $D$, and repeated indices are summed. Inserting this de-
composition of $S$ into (1) and expanding $e^{-\delta S/\hbar}$ in a power series yields the semiclassical
expansion of $Z(\beta)$:
\[ Z(\beta) = \int_{\mathbb{R}^D} d^D x_0 \, e^{-S[x_0] / h} \int_{u(0) = 0}^{u(\beta h) = 0} [D u(\tau)] \, e^{-S_2[u] / h} \sum_{n=0}^{\infty} \frac{1}{n!} \left( -\frac{\delta S[u]}{h} \right)^n. \] (4)

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

\[ Z_2(\beta) \equiv \int_{\mathbb{R}^D} d^D x_0 \, e^{-S[x_0] / h} \int_{u(0) = 0}^{u(\beta h) = 0} [D u(\tau)] \, e^{-S_2[u] / h} \]
\[ = \int_{\mathbb{R}^D} d^D x_0 \, e^{-S[x_0] / h} \Delta^{-1/2}, \] (5)

where \( \Delta \) is the determinant of the fluctuation operator \( F \):

\[ \Delta = \text{Det} \, F, \quad F_{ij} = -m \frac{d^2}{d\tau_2} \delta_{ij} + \partial_i \partial_j V(x_c). \] (6)

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

\[ \langle u_{i_1}(\tau_1) \ldots u_{i_k}(\tau_k) \rangle \equiv \int_{u(0) = 0}^{u(\beta h) = 0} [D u(\tau)] \, e^{-S_2[u] / h} \, u_{i_1}(\tau_1) \ldots u_{i_k}(\tau_k). \] (7)

Since the action \( S_2[u] \) is quadratic, one can show that

\[ \langle u_{i_1}(\tau_1) \ldots u_{i_k}(\tau_k) \rangle = \hbar^{k/2} \Delta^{-1/2} \sum_P G_{i_1 i_2}(\tau_{j_1}, \tau_{j_2}) \ldots G_{i_{k-1} i_k}(\tau_{j_{k-1}}, \tau_{j_k}), \] (8)

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

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

satisfying the boundary conditions

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

In the Appendix we present a recipe for obtaining \( \Delta \) 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 the previous section, let us apply it to the case of central potentials, i.e., \( V = V(r) \), where \( r \equiv |x| \). First of all, we note that, because of the radial symmetry, \( \rho(\beta; x_0, x_0) \) can only depend on \( r_0 = |x_0| \). Thus, without loss of generality, we may take \( x_0 = r_0 \, e_1 \), where \( e_1 \) is the unit vector pointing in the \( x_1 \)-direction, and perform the angular integration in (13) to obtain

\[ Z(\beta) = \frac{2\pi^{D/2}}{\Gamma(D/2)} \int_0^{\infty} dr_0 \, r_0^{D-1} \, \rho(\beta; r_0 \, e_1; r_0 \, e_1). \] (11)
In general, there are many classical trajectories satisfying the boundary conditions \( x(0) = \mathbf{x}(\beta h) = r_0 \mathbf{e}_1 \). 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. Besides, 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, \( x_c(\tau) = r_c(\tau) \mathbf{e}_1 \), the fluctuation operator \( F \) is diagonal in the indices \( i,j \). Indeed, since \( V = V(r) \), we have

\[
\partial_i \partial_j V(r) = \frac{V''(r)}{r} \delta_{ij} + \left[ V''(r) - \frac{V'(r)}{r} \right] \frac{x_i x_j}{r^2},
\]

(12)

which, for \( x_i = r \delta_{i1} \), gives \( \partial_i \partial_1 V(r_c) = V''(r_c), \partial_i \partial_1 V(r_c) = r_c^{-1} V'(r_c) \) for \( i = 2, \ldots, D \), and \( \partial_i \partial_j V(r_c) = 0 \) if \( i \neq j \). Thus, \( \Delta = \Delta_\ell \Delta_t^{D-1} \), where

\[
\Delta_\ell = \text{Det} \left[ -m \partial_\tau^2 + V''(r_c) \right], \quad \Delta_t = \text{Det} \left[ -m \partial_\tau^2 + r_c^{-1} V'(r_c) \right]
\]

(13)

(\( \ell \) and \( t \) stand for longitudinal and transverse, respectively).

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

\[
[-m \partial_\tau^2 + V''(r_c)] G_\ell(\tau, \tau') = \delta(\tau - \tau'),
\]

(14a)

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

(14b)

\( \Delta_\ell \) and \( G_{\ell}(\tau, \tau') \) 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. [3]. There, the following results were derived:

\[
\Delta_\ell = \frac{2\pi \hbar}{m} \Omega_\ell(0, \beta h), \quad G_{\ell}(\tau, \tau') = \frac{\Omega_\ell(0, \tau_<) \Omega_\ell(\tau_>, \beta h)}{m \Omega_\ell(0, \beta h)}.
\]

(15)

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

\[
\Omega_\ell(\tau, \tau') \equiv \frac{\eta_a(\tau) \eta_b(\tau') - \eta_a(\tau') \eta_b(\tau)}{\eta_a(\tau') \eta_b(\tau) - \eta_a(\tau) \eta_b(\tau')}.
\]

(16)

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

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

(17)

By differentiating the equation of motion \( m \ddot{r}_c - V'(r_c) = 0 \) with respect to \( \tau \), one can verify that \( \eta_a(\tau) = \dot{r}_c(\tau) \) is one such solution. The other can be taken as \( \eta_b(\tau) = \dot{r}_c(\tau) \int_0^\tau d\tau' [\dot{r}_c(\tau')]^{-2} \). For such a choice, the denominator of \( \Omega_\ell(\tau, \tau') \) is equal to 1 and, since \( \eta_b(0) = 0 \), one has \( \Delta_\ell = (2\pi \hbar/m) \eta_a(0) \eta_b(\beta h) \). Because of these simplifying features, we shall refer to those solutions as the “canonical” solutions of (14).

In order to obtain \( \Delta_t \) and \( G_t(\tau, \tau') \) one simply replaces \( \Omega_\ell(\tau, \tau') \) in (13) by
\[\Omega_{\ell}(\tau, \tau') \equiv \frac{\varphi_a(\tau) \varphi_b(\tau') - \varphi_a(\tau') \varphi_b(\tau)}{\varphi_a(\tau') \dot{\varphi}_b(\tau') - \dot{\varphi}_a(\tau') \varphi_b(\tau')} ,\]  

(18)

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

\[[-m \partial^2_\tau + r_c^{-1} V'(r_c)] \varphi(\tau) = 0 .\]  

(19)

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

III. APPLICATIONS

Using the results of the previous section we may write the quadratic approximation to the partition function as

\[Z_2(\beta) = \frac{2\pi^{D/2}}{\Gamma(D/2)} \int_0^\infty dr_0 r_0^{D-1} e^{-\frac{S[x_c]}{\hbar}} \left(\Delta_t \Delta_t^{-1}\right)^{-1/2} .\]  

(20)

It can be readily calculated from the knowledge of \(x_c(\tau)\) alone. This will be accomplished below for both the harmonic and single-well quartic anharmonic oscillators.

A. The harmonic oscillator

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

\[V(r) = \frac{1}{2} m\omega^2 r^2 .\]  

(21)

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

\[Z(\beta) = \frac{2\pi^{D/2}}{\Gamma(D/2)} \int_0^\infty dr_0 r_0^{D-1} e^{-\frac{S[x_c]}{\hbar}} \Delta_{\ell}^{-D/2} .\]  

(22)

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

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

(23)

The classical action can be readily computed, giving

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

(24)

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

\[\Delta_{\ell} = \frac{2\pi \hbar \sinh(\beta\hbar\omega)}{m\omega} .\]  

(25)

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

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

(26)

which is the well-known result for the partition function of the \(D\)-dimensional harmonic oscillator.
B. The single-well quartic anharmonic oscillator

Let us now consider the potential

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

(27)

In order to simplify notation, it is convenient to replace \( r \) and \( \tau \) 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

\[ \frac{d^2 q}{d\theta^2} = q + q^3 , \]  

(28)

whose solution, taking into account the boundary conditions, is

\[ q_c(\theta) = q_t \text{ nc}(u_\theta, k) , \]  

(29)

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

\[ u_\theta = \sqrt{1 + q^2_t} \left( \theta - \frac{\Theta}{2} \right) , \quad k = \sqrt{\frac{2 + q^2_t}{2(1 + q^2_t)}} , \]  

(30)

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

\[ q_0 = q_c(\Theta) = q_t \text{ nc} u_\Theta . \]  

(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

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

(32)

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

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

(33)

Performing the integration and using (31) yields

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

(34)

where \( E(\varphi, k) \) denotes the Elliptic Integral of the Second Kind and \( \varphi_\Theta \equiv \arccos[q_c(\theta)/q_0] = \arccos(cn u_\theta) \).

The canonical solutions of (17) and (19) are given by
\[ \eta_a(\theta) = \omega q_t \sqrt{1 + q_t^2} \frac{\text{sn} u_\theta \text{dn} u_\theta}{\text{cn}^2 u_\theta}, \]  
\[ \eta_b(\theta) = \frac{1}{\omega^2 q_t (1 + q_t^2)} \frac{\text{sn} u_\theta \text{dn} u_\theta}{\text{cn}^2 u_\theta} \left[ \frac{k^2 - 1}{k^2} u_\theta + \frac{1 - 2k^2}{k^2} \text{E}(\varphi_\theta, k) \right. \]  
\[ - \frac{\text{cn} u_\theta \text{dn} u_\theta}{\text{sn} u_\theta} + (k^2 - 1) \frac{\text{sn} u_\theta \text{cn} u_\theta}{\text{dn} u_\theta} - (\theta \to 0) \left] , \right. \]  
\[ \varphi_a(\theta) = q_t \text{nc} u_\theta , \]  
\[ \varphi_b(\theta) = \frac{\text{nc} u_\theta}{\omega k^2 q_t \sqrt{1 + q_t^2}} \left[ \text{E}(\varphi_\theta, k) + (k^2 - 1) u_\theta - (\theta \to 0) \right] . \]  

Thus,
\[ \Delta_\ell = \frac{4\pi \hbar}{m\omega} \frac{\text{sn}^2 u_\theta \text{dn}^2 u_\theta}{\sqrt{1 + q_t^2} \text{cn}^4 u_\theta} \left[ \frac{1 - k^2}{k^2} u_\theta + \frac{2k^2 - 1}{k^2} \text{E}(\varphi_\theta, k) \right. \]  
\[ + \frac{\text{cn} u_\theta \text{dn} u_\theta}{\text{sn} u_\theta} + (1 - k^2) \frac{\text{sn} u_\theta \text{cn} u_\theta}{\text{dn} u_\theta} \right] , \]  
\[ \Delta_t = \frac{4\pi \hbar}{m\omega} \frac{\text{nc}^2 u_\theta}{k^2 \sqrt{1 + q_t^2}} \left[ \text{E}(\varphi_\theta, k) + (k^2 - 1) u_\theta \right] . \]  

We now have all the necessary ingredients to compute the quadratic approximation to \( Z(\beta) \):
\[ Z_2(\beta) = \frac{2\pi^{D/2}}{\Gamma(D/2)} \left( \frac{m\omega^2}{\lambda} \right)^{D/2} \int_0^\infty dq_0 q_0^{D-1} e^{-I[q_0]/g} \left( \Delta_\ell \Delta_t^{D-1} \right)^{-1/2} , \]  
where \( g \equiv \hbar \lambda / m^2 \omega^3 \). However, to perform the integral over \( q_0 \) one must write \( I[q_c], \Delta_\ell \) and \( \Delta_t \) in terms of \( q_0 \). In view of Eq. \( (31) \), it is much simpler to change the variable of integration from \( q_0 \) to \( q_t \):
\[ Z_2(\beta) = \frac{2\pi^{D/2}}{\Gamma(D/2)} \left( \frac{m\omega^2}{\lambda} \right)^{D/2} \int_0^{q_\Theta} dq_t \left( \frac{\partial q_0}{\partial q_t} \right)_{\Theta} (q_t \text{nc} u_\Theta)^{D-1} e^{-I[q_\Theta]/g} \left( \Delta_\ell \Delta_t^{D-1} \right)^{-1/2} , \]  
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 \( (31) \) by differentiation or, more simply, by using the identity \[ (39) \]
\[ \left( \frac{\partial q_0}{\partial q_t} \right)_{\Theta} = \frac{m\omega}{4\pi \hbar} \frac{U'(q_t) \Delta_\ell}{\sqrt{2 [U(q_0) - U(q_t)]}} . \]  

As an application, we may use \( (38) \) to calculate the specific heat of the \( D \)-dimensional single-well quartic anharmonic oscillator, given by
\[ C = \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z . \]
Using the program MAPLE, we computed this expression for a few values of the temperature $[7]$. 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

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

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

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

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

**IV. CONCLUSIONS**

The results of the previous sections confirm the findings of references $[8,9]$, 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 with 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 “quasi-exact”. By contrast, the semiclassical approach directly approximates the whole sum. Its lowest order agrees well with the quasi-exact 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 WKB, 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 WKB approximates each term in the sum; but 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 (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 $\beta$ and $r_0$, the number of classical paths may be two, one or zero. Besides, 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 [13]. 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 non-trivial 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 A:

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

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

satisfying the initial conditions
The function is known as the Jacobi commutator \([A][2]\). It can be explicitly constructed as follows. Let \(x(\tau; a, b)\) be the solution of the equation of motion \([3]\) satisfying the initial conditions \(x(0) = a, \dot{x}(0) = b\). Let \(A\) and \(B\) be the \(D \times D\) matrices defined as

\[
A_{jk}(\tau) = \frac{\partial}{\partial a_k} x_j(\tau; a = x_0, b = v_0), \\
B_{jk}(\tau) = \frac{\partial}{\partial b_k} x_j(\tau; a = x_0, b = v_0),
\]

where \(v_0 = \dot{x}_c(0)\). By differentiating Eq. \((2)\) with respect to \(a_k\) and \(b_k\) (and taking \(a = x_0, b = v_0\), one can show that they are solutions of \((A1)\). They are also invertible for \(\tau\) small enough \([20]\) (but not zero). Indeed, \(x(\tau) = a + b\tau + O(\tau^2)\) when \(\tau \to 0\), hence \(A(\tau) = \mathbb{I} + O(\tau^2)\) and \(B(\tau) = \tau \mathbb{I} + O(\tau^2)\). Therefore, the expression

\[
J(\tau, \tau') = -\frac{1}{m} \left[ A(\tau) A^{-1}(\tau') - B(\tau) B^{-1}(\tau') \right] \left[ \dot{A}(\tau') A^{-1}(\tau') - \dot{B}(\tau') B^{-1}(\tau') \right]^{-1}
\]

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

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

\[
G(\tau, \tau') = J(\tau, 0) M(0, \beta h) J(\beta h, \tau') - J(\tau, \beta h) M(\beta h, 0) J(0, \tau') \theta(\tau - \tau') ,
\]

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

\[
J(\tau, 0) M(0, \beta h) J(\beta h, \tau') + J(\tau, \beta h) M(\beta h, 0) J(0, \tau') = -J(\tau, \tau') ,
\]

\[
\partial_\tau J(\tau, 0) M(0, \beta h) J(\beta h, \tau) + \partial_\tau J(\tau, \beta h) M(\beta h, 0) J(0, \tau) = \frac{1}{m} \mathbb{I}.
\]

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

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

\[
G(\tau' + 0, \tau') = G(\tau' - 0, \tau')
\]

[use \((A7)\) with \(\tau = \tau'\)], and (iv) its derivative with respect to \(\tau\) has the discontinuity implied by \((\beta)\),

\[
\frac{\partial}{\partial \tau} G(\tau = \tau' + 0, \tau') - \frac{\partial}{\partial \tau} G(\tau = \tau' - 0, \tau') = -\frac{1}{m} \mathbb{I}
\]

[use \((A8)\)].

Finally, the determinant \(\Delta\) of the fluctuation operator \(\mathcal{F}\) is given by

\[
\Delta = (2\pi h)^D \det [-J(\beta h, 0)].
\]

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

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[1] R. P. Feynman and A. R. Hibbs, Quantum Mechanics and Path Integrals (McGraw-Hill, New York, 1965); R. P. Feynman, Statistical Mechanics (Addison-Wesley, New York, 1972).
[2] L. S. Schulman, Techniques and Applications of Path Integration (John Wiley, New York, 1981).
[3] H. Kleinert, Path Integrals in Quantum Mechanics, Statistics and Polymer Physics (World Scientific, Singapore, 1995).
[4] F. W. Wiegel, Introduction to Path-Integral Methods in Physics and Polymer Science (World Scientific, Singapore, 1986).
[5] M. C. Gutzwiller, Chaos in Classical and Quantum Mechanics (Springer-Verlag, New York, 1990).
[6] M. Berry, Some quantum-to-classical asymptotics, in Chaos and Quantum Physics, edited by M.-J. Giannoni, A. Voros, and J. Zinn-Justin (North-Holland, Amsterdam, 1991).
[7] This is to be contrasted with the semiclassical approximation in Quantum Mechanics, where one has to find all the stationary points of the action, irrespective of being minima, maxima or points of inflection.
[8] C. A. A. de Carvalho, R. M. Cavalcanti, E. S. Fraga, and S. E. Jorás, Ann. Phys. (N.Y.) 273, 146 (1999).
[9] C. A. A. de Carvalho and R. M. Cavalcanti, in Trends in Theoretical Physics II (AIP Conference Proceedings 484), edited by H. Falomir, R. E. Gamboa Saravi, and F. A. Schaposnik (AIP, Woodbury, 1999); quant-ph/9903028.
[10] F. Vinette and J. Čižek, J. Math. Phys. 32, 3392 (1991); W. Janke and H. Kleinert, Phys. Rev. Lett. 75, 2787 (1995).
[11] C. DeWitt-Morette, Comm. Math. Phys. 28, 47 (1972); 37, 63 (1974); Ann. Phys. (N.Y.) 97, 367 (1976).
[12] Maurice M. Mizrahi, J. Math. Phys. 17, 566 (1976); 19, 298 (1978); 20, 844 (1979).
[13] I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series, and Products (Academic Press, New York, 1965).
[14] P. F. Byrd and M. D. Friedman, Handbook of Elliptic Integrals for Engineers and Physicists (Springer-Verlag, Berlin, 1954).
[15] M. Abramowitz and I. A. Stegun (eds.), Handbook of Mathematical Functions (Dover, New York, 1965).
[16] This definition only makes sense for \( \tau < \beta \hbar / 2 \). For \( \tau > \beta \hbar / 2 \) one must take

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

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

[17] In order to compute the derivative in (40), we have approximated \( \ln Z \) by a rational function using Thiele’s interpolation formula. See [15], formula 25.2.50.

[18] For instance, when \( g = 0.2 \) Eq. (42) gives values of \( E_0, E_1 \) and \( E_9 \) that differ from the exact ones by less than 3%, 1% and 0.1%, respectively.

[19] L. S. Schulman and R. W. Ziolkowski, *Path integral asymptotics in the absence of classical paths*, in *Path Integrals from mev to Mev*, edited by V. Sakyankit et al (World Scientific, Singapore, 1989).

[20] We conjecture that they are in fact invertible for any \( \tau \in (0, \beta \hbar) \), except maybe for a finite number of points.

[21] S. Coleman, *The uses of instantons*, in *The Whys of Subnuclear Physics*, edited by A. Zichichi (Plenum, New York, 1979); reproduced in S. Coleman, *Aspects of Symmetry* (Cambridge University Press, Cambridge, 1985).
FIGURES

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

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). $g \equiv \hbar \lambda/m^2 \omega^3 = 0.2$. 
