Semiclassical Series at Finite Temperature

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Abstract

We derive the semiclassical series for the partition function of a one-dimensional quantum-mechanical system consisting of a particle in a single-well potential. We do this by applying the method of steepest descent to the path-integral representation of the partition function, and we present a systematic procedure to generate the terms of the series using the minima of the Euclidean action as the only input. For the particular case of a quartic anharmonic oscillator, we compute the first two terms of the series, and investigate their high and low temperature limits. We also exhibit the non-perturbative character of the terms, as each corresponds to sums over infinite subsets of perturbative graphs. We illustrate the power of such resummations by extracting from the first term an accurate nonperturbative estimate of the ground-state energy of the system and a curve for the specific heat. We conclude by pointing out possible extensions of our results which include field theories with spherically symmetric classical solutions.

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I. INTRODUCTION

Semiclassical series were introduced in Quantum Mechanics by the pioneering works of Brillouin [1], Kramers [2] and Wentzel [3]. In order to solve the time-independent Schrödinger equation for slowly-varying potentials, they proposed an ansatz for the wavefunction of the form (here particularized to one dimension)

$$\psi(x) = e^{iS(x)/\hbar},$$

(1)

that led to a Ricatti equation for $S(x)$. The assumption of slow variation of the potential allowed for an iterative procedure in solving that equation. As a result, one obtained a series expansion of $S(x)$ in powers of $\hbar$, i.e., $S(x) = \sum_{n=0}^{\infty} S_n(x)\hbar^n$, with $S_{n+1}(x)$ given in terms of $S_n(x)$ by means of a recursion relation, and $S_0(x)$ satisfying the Hamilton-Jacobi equation for a particle with the same energy and external potential as those of the Schrödinger equation. Thus, the zeroth order approximation could be associated to a classical path, from an arbitrary $x_0$ to $x$, whose classical action $S_0(x) = S_{cl}(x_0 \to x)$, apart from a sign, should be used in (1). The choice of $x_0$ just fixed a normalization constant.

The terms of the series derived in references [1–3] were plagued with divergences that occurred at the turning points of the classical motion, a problem that came to be known as the connection problem. Dunham [4] bypassed this difficulty by turning $x$ into a complex variable $z$, and using different linear combinations of $e^{\pm iS(x)/\hbar}$ as asymptotic series for $\psi(x)$ along the real axis. Assuming a potential with only two classical turning points $x_a$ and $x_b$ ($x_a < x_b$), three different linear combinations should be used as $x < x_a$, $x_a < x < x_b$ or $x > x_b$. Demanding that $\psi(z)$ be real, bounded and single-valued on the real axis, and writing $S(z) = \int p(z') dz'$, he could arrive at the quantization condition

$$\oint p(z)dz = 2\pi n\hbar \quad (n = 1, 2, \ldots),$$

(2)

for any closed contour encircling the segment $(x_a, x_b)$. The semiclassical series for $\psi(z)$ led to semiclassical series for $S(z)$ and $p(z)$ which, together with (2), provided an expression for the energy levels as a power series in $\hbar$, generalizing the Bohr-Sommerfeld condition. That series was used as a starting point for the works of Bender, Olaussen and Wang [5] and Balian, Parisi and Voros [6,7], who refined such asymptotic representations to obtain highly accurate estimates of the energy levels of the single-well quartic anharmonic oscillator. These could be compared to the estimates obtained by Bender and Wu [8–10] from the investigation of the large order behavior of perturbation theory [11–14].

Apart from energy eigenfunctions and eigenvalues, semiclassical series were also written down for Green’s functions by Balian and Bloch [15]. Defining the resolvent operator $\hat{G}$ through

$$(\hat{H} - z) \hat{G} = \mathbb{I}$$

(3)

for a complex energy $z$, $\hat{H}$ being the Hamiltonian of the system, they used an ansatz of the form

$$G(x, x'; z) = A(x, x') e^{S(x, x'; z)/\hbar}. \quad (4)$$
From the defining equation (3), under assumptions similar to those in the first paragraph, they started from zeroth order estimates $S_0(x, x'; z)$ and $A_0(x, x')$ by neglecting nonleading terms in $\hbar$. They found that $S_0$ satisfied a Hamilton-Jacobi equation for complex energy $z$, solved by a classical trajectory from $x$ to $x'$. The amplitude $A_0(x, x')$ turned out to be related to derivatives of the classical $S_0$. Just as before, the zeroth estimates could be used to generate a whole series expansion by an iterative procedure. Note that $z = E + i\gamma$, the analytic continuation to complex energies being used to circumvent problems with singularities (turning points in one dimension; caustics in higher dimensions).

In all the discussions mentioned, the first term of the semiclassical series was obtained from quantities related to some classical trajectory. Path integral representations for correlation functions [16–20], which sum over trajectories, should therefore provide a natural setting to derive semiclassical series. Indeed, approximating quantum-mechanical path integrals by the stationary phase method leads to zeroth order estimates given by the paths that solve the classical equations of motion, the saddle points of the action functional. Thus,

$$
\langle x | e^{-i\frac{\hat{H}}{\hbar}(t-t')} | x' \rangle = \int_{x(t')=x'}^{x(t)=x} [Dx(t)] \ e^{iS[x(t)]/\hbar},
$$

may be time Fourier transformed to yield (4). The saddle-point contribution, and fluctuations around it, will yield the zeroth order estimates $S_0$ and $A_0$ mentioned before.

Although semiclassical quantization by means of path integrals became widely used, as evidenced by Gutzwiller’s work [21], and by extensions to field theories by Dashen, Hasslacher and Neveu [22–25], almost all discussions never went beyond the first term of a semiclassical series. Notable exceptions were the works of DeWitt-Morette [26], for arbitrary potentials in Quantum Mechanics, and Mizrahi [27], for the single-well quartic anharmonic oscillator in Quantum Mechanics (more recently [28], a derivation of the higher order terms of the series using transport-type recurrence equations also became available). However, these contributions to the mathematical physics literature did not receive the attention they certainly deserved in more applied work. We were no exception, and only became aware of these articles after we had rederived the semiclassical series using the methods of section II.

Semiclassical methods for finite temperature field theories [29–31] also remained restricted to derivations of the first term of a semiclassical series [32], even when the problem was reduced to Quantum Statistical Mechanics [33,34], viewed as field theory at a point (zero spatial dimension). Some references resorted to extensions to the complex plane [35–37] to include complex paths required to describe Fourier transformed quantities but, again, those treatments were not concerned with obtaining the whole series.

The central objective of the present article is to bridge this gap. Thus, we undertook the task of finding a systematic path integral procedure to generate a semiclassical series for Quantum Statistical Mechanics which led us to the construction of each term of the series from the knowledge of the solution(s) of the classical equations of motion. We concentrated our attention on the partition function, for which use of the method of steepest descent only required real solutions as saddle-points [38]. The restriction of our analysis to one-dimensional quantum-mechanical systems (i.e., scalar field theories at a point and at finite temperature) allowed us to construct the semiclassical propagator needed to generate the terms of the series.
This article is organized as follows: section II presents the derivation of the semiclassical series for a generic potential of the single-well type, both in quantum-mechanical language and in field-theoretic language, the latter allowing for a simple connection with the works of references [26,27]. It should be remarked, however, that our presentation is quite simple, being a natural extension of textbook material [14], and having profited greatly from the clear account of reference [37]. To emphasize that our construction is free of turning-point singularities, details of the derivation were worked out in Appendices A and B; section III discusses the single-well quartic anharmonic oscillator. There, we constructed the two first terms of the series explicitly, and looked at relevant limits. We also computed the ground-state energy and the specific heat, as illustrations. Appendices C, D and E complement the calculations in the text; section IV presents our conclusions, points out directions for future work, and lists a number of situations where our results could be applied.

II. STATISTICAL MECHANICS

A. Quantum-mechanical path integrals

The partition function for a one-dimensional quantum-mechanical system consisting of a particle of mass $m$ in the presence of a potential $V(x)$ in equilibrium at inverse temperature $\beta$ can be written as a path integral:

$$Z(\beta) = \int_{-\infty}^{\infty} dx_0 \int_{x(0)=x_0}^{x(\beta\hbar)=x_0} [Dx(\tau)] e^{-S/\hbar},$$  \hspace{1cm} (6)

$$S[x] = \int_0^{\beta\hbar} d\tau \left[ \frac{1}{2} m \left( \frac{dx}{d\tau} \right)^2 + V(x) \right].$$  \hspace{1cm} (7)

For convenience we define the dimensionless quantities $q \equiv x/x_N$, $\theta \equiv \omega_N \tau$, $\Theta \equiv \beta \hbar \omega_N$, $U(q) \equiv V(x_Nq)/m \omega_N^2 x_N^2$ and $g \equiv \hbar/m \omega_N x_N^2$, where $\omega_N^{-1}$ and $x_N$ are natural time and length scales of the problem, respectively. In terms of these quantities we rewrite the partition function as

$$Z(\Theta) = \int_{-\infty}^{\infty} dq_0 \int_{q(0)=q_0}^{q(\Theta)=q_0} [Dq(\theta)] e^{-I/g},$$  \hspace{1cm} (8)

$$I[q] = \int_0^{\Theta} d\theta \left[ \frac{1}{2} \dot{q}^2 + U(q) \right],$$  \hspace{1cm} (9)

where the dot denotes differentiation in $\theta$.

We generate a semiclassical series for $Z(\Theta)$ by: (i) finding the minima $q_c(\theta)$ of the Euclidean action $I$, i.e., the stable classical paths that solve the Euler-Lagrange equation of motion, subject to the boundary conditions; (ii) expanding the Euclidean action around these classical paths; (iii) deriving a quadratic semiclassical propagator by neglecting terms higher than second order in the expansion; (iv) using that propagator to compute higher (than quadratic) order contributions perturbatively.
For the sake of simplicity, we shall restrict our analysis to potentials of the single-well type, twice differentiable, and such that \( U'(q) = 0 \) only at the minimum of \( U \), which we shall assume to be at the origin (see Fig. 1). This guarantees that, given \( q_0 \) and \( \Theta \), there will be a unique classical path satisfying the boundary conditions. Multiple-well potentials force us to consider more than one classical path for certain choices of \( q_0 \) and \( \Theta \). This phenomenon has been analyzed, for a double-well type potential, using the language of catastrophes and bifurcations. Semiclassical series for the double-well quartic oscillator will be presented elsewhere.

The Euler-Lagrange equation
\[
\ddot{q} - U'(q) = 0,
\]
subject to the boundary conditions \( q(0) = q(\Theta) = q_0 \), describes the motion of a particle in the potential \( \text{minus} \ U \). Its first integral is
\[
\frac{1}{2} \dot{q}^2 = U(q) - U(q_t),
\]
where \( q_t \) denotes the single turning point (since we have an inverted single well) of the motion, defined implicitly by
\[
\Theta = 2 \int_{q_0}^{q_t} dq/v(q,q_t),
\]
where \( v(q,q') \equiv \text{sign}(q' - q) \sqrt{2[U(q) - U(q')]}, \) and equation (12) is a consequence of integrating (11). Thus, for a single well, given \( q_0 \) and \( \Theta \), the classical path will go from \( q_0 \), at \( \theta = 0 \), to \( q_t = q_t(q_0,\Theta) \), at \( \theta = \Theta/2 \), and return to \( q_0 \) at \( \theta = \Theta \). (Note that \( \text{sign}(q_t) = \text{sign}(q_0) \).)

The action for this classical path has a simple expression in terms of its turning point:
\[
I[q_c] = \Theta U(q_t) + 2 \int_{q_0}^{q_t} dq U(q,q_t),
\]
where we have used (11). The first term in (13) corresponds to the high-temperature limit of \( Z(\Theta) \), where classical paths collapse to a point \( (q_t \rightarrow q_0) \). The last term will be negligible for potentials that vary little over a thermal wavelength \( \lambda = h \sqrt{\beta/m} \). However, by decreasing the temperature it will become important and bring in quantum effects.

We now expand the action around the classical path. Letting \( q(\theta) = q_c(\theta) + \eta(\theta) \), with \( \eta(0) = \eta(\Theta) = 0 \), we obtain
\[
I[q] = I[q_c] + I_2[\eta] + \delta I[\eta],
\]
where
\[
I_2[\eta] \equiv \frac{1}{2} \int_0^\Theta d\theta \left\{ \dot{\eta}^2(\theta) + U''[q_c(\theta)] \eta^2(\theta) \right\},
\]
\[
\delta I[\eta] \equiv \int_0^\Theta d\theta \delta U(\theta, \eta) = \sum_{n=3}^{\infty} \frac{1}{n!} \int_0^\Theta d\theta U^{(n)}[q_c(\theta)] \eta^n(\theta).
\]
Inserting (14) into (8) and expanding $e^{-\delta I/g}$ in a power series yields

$$Z(\Theta) = \int_{-\infty}^{\infty} dq_0 \exp \left[ -I(q_0)/g \right] \exp \left[ -I[\eta(\theta)]/g \right] \sum_{m=0}^{\infty} \frac{1}{m!} \left( -\frac{\delta I[\eta]}{g} \right)^m .$$

(17)

If we interchange, à la Feynman [16], the integral over deviations from the classical path with the integrals over various times $\{\theta_i\}$, coming from insertions of (13), we break up the path-integral into pieces which go from zero to the various $\theta_i$ and, finally, to $\Theta$. Thus,

$$Z(\Theta) = \int_{-\infty}^{\infty} dq_0 \exp \left[ -I(q_0)/g \right] \left[ G_c(0, 0; \Theta, 0) + \sum_{n=1}^{\infty} \frac{(-1)^n}{g^n n!} G_n(q_0, \Theta) \right],$$

(18)

$$G_n(q_0, \Theta) = \left( \prod_{j=1}^{n} \int_{0}^{\Theta} d\theta_j \int_{-\infty}^{\infty} d\eta_j \right) G_c(0, 0; \theta_1, \eta_1) \delta U(\theta_1, \eta_1)$$

$$\times G_c(\theta_1, \eta_1; \theta_2, \eta_2) \cdots \delta U(\theta_n, \eta_n) G_c(\theta_n, \eta_n; \Theta, 0) \right|_{\theta_1 \leq \theta_2 \leq \cdots \leq \theta_n} ,$$

(19)

with $G_c(\theta_1, \eta_1; \theta_2, \eta_2)$, the semiclassical propagator, emerging naturally from doing the path-integral in each piece:

$$G_c(\theta_1, \eta_1; \theta_2, \eta_2) = \int_{\eta(\theta_1) = \eta_1}^{\eta(\theta_2) = \eta_2} [D\eta(\theta)] \exp \left[ -I_2[\eta_1, \theta_2; \eta] \right],$$

(20)

$$I_2[\theta_1, \theta_2; \eta] = \frac{1}{2} \int_{\theta_1}^{\theta_2} d\theta \left\{ \dot{\eta}^2 + U''[q_c(\theta)] \eta^2 \right\} .$$

(21)

It remains to show how one can obtain that propagator from the knowledge of the classical path. This is the central point in the whole procedure. For this, we use the fact that the action $I_2$ is quadratic in $\eta$, and so the path integral in (20) is completely determined by the extremum $\eta_c(\theta)$ of $I_2[\theta_1, \theta_2; \eta]$, which satisfies

$$\ddot{\eta} - U''[q_c(\theta)] \eta = 0 ,$$

(22)

subject to the boundary conditions $\eta(\theta_1) = \eta_1$ and $\eta(\theta_2) = \eta_2$. Thus,

$$G_c(\theta_1, \eta_1; \theta_2, \eta_2) = G_c(\theta_1, 0; \theta_2, 0) \exp \left[ -I_2[\theta_1, \theta_2; \eta_c] \right],$$

(23)

where, after an integration by parts,

$$I_2[\theta_1, \theta_2; \eta_c] = \frac{1}{2} \left[ \eta_2 \dot{\eta}_c(\theta_2) - \eta_1 \dot{\eta}_c(\theta_1) \right].$$

(24)

We can obtain $\eta_c(\theta)$ by finding the linear combination of any two linearly independent solutions, $\eta_a(\theta)$ and $\eta_b(\theta)$, of (22) which satisfies $\eta_c(\theta_1) = \eta_1$ and $\eta_c(\theta_2) = \eta_2$. The result is

$$\eta_c(\theta) = \frac{\eta_1 \Omega(\theta, \theta_2) + \eta_2 \Omega(\theta_1, \theta)}{\Omega(\theta_1, \theta_2)} ,$$

(25)
where
\[ \Omega(\theta, \theta') \equiv \eta_a(\theta) \eta_b(\theta') - \eta_a(\theta') \eta_b(\theta). \] (26)

We may then write
\[ I_2[\theta_1, \theta_2; \eta_c] = \frac{1}{2 \Omega_{12}} [W_{12} \eta_2^2 + W_{21} \eta_1^2 - (W_{11} + W_{22}) \eta_1 \eta_2], \] (27)

where \( \Omega_{ij} \equiv \Omega(i, j) \) and \( W_{ij} \equiv \partial \Omega_{ij} / \partial \theta_j \). (Note that \( W_{ii} \) is the Wronskian of \( \eta_a \) and \( \eta_b \) computed at \( \theta_i \).)

Explicit expressions for \( \eta_a(\theta) \) and \( \eta_b(\theta) \) can be obtained as follows. By differentiating (10) with respect to \( \theta \), one can verify that \( \eta_a(\theta) = \dot{q}_c(\theta) \) satisfies (22). For the second solution, we take \( \eta_b(\theta) = \dot{q}_c(\theta) Q(\theta) \), where \( Q(\theta) \) is defined as
\[ Q(\theta) = Q(0) + \int_0^\theta \frac{d\theta'}{\dot{q}_c^2(\theta')} \] (28)

for \( \theta < \Theta/2 \), \( Q(\theta) = -Q(\Theta - \theta) \) for \( \theta > \Theta/2 \), and \( Q(0) \) is chosen so as to make \( \dot{q}_b(\theta) \) continuous at \( \theta = \Theta/2 \) (see Appendix A). One can easily check, using (11), that \( \eta_b(\theta) \) indeed satisfies (22). (Alternatively, one could use a procedure introduced by Cauchy \[26,27\], and differentiate the classical solution \( q_c(\theta) \) with respect to any two parameters related to its two constants of integration.) We can now write explicit expressions for \( \Omega_{12} \) and \( W_{ij} \):
\[ \Omega_{12} = \dot{q}_c(\theta_1) \dot{q}_c(\theta_2) [Q(\theta_2) - Q(\theta_1)], \] (29)
\[ W_{ij} = \dot{q}_c(\theta_i) U''[q_c(\theta_j)] [Q(\theta_j) - Q(\theta_i)] + \frac{\dot{q}_c(\theta_i)}{\dot{q}_c(\theta_j)}. \] (30)

As a final step, the pre-factor in (23) is derived in Appendix B, using the methods of Refs. \[14,37\]. The result is
\[ G_c(\theta_1, 0; \theta_2, 0) = \left[ \frac{W_{11}}{2\pi g \Omega_{12}} \right]^{1/2}. \] (31)

From (30), one easily finds \( W_{ii} = 1 \). Therefore, our quadratic semiclassical propagator is given by
\[ G_c(\theta_1, \eta_1; \theta_2, \eta_2) = \frac{1}{\sqrt{2\pi g \Omega_{12}}} \exp \left[ -\frac{1}{2g \Omega_{12}} (W_{12} \eta_2^2 + W_{21} \eta_1^2 - 2 \eta_1 \eta_2) \right]. \] (32)

As promised, it is completely determined by the classical solution.

Finally, we note that the van Vleck determinant \( \Delta \) is a by-product of (32):
\[ \Delta(q_0, \Theta) = G_c^{-2}(0, 0; \Theta, 0) = 2\pi g \Omega(0, \Theta) = 4\pi g \dot{q}_c^2(0) Q(0). \] (33)

Using (11) and (17) one can express \( \Delta \) as
\[ \Delta = \frac{4\pi g [U(q_t) - U(q_0)]}{U''(q_t)} \left( \frac{\partial \Theta}{\partial q_t} \right)_{q_0}. \] (34)

Together with (13), this shows that one does not need to know \( q_c(\theta) \) in order to write the first term in the semiclassical series (18); it is enough to know \( q_t(q_0, \Theta) \).
B. Field-theoretic approach

We may generate the semiclassical series in an alternative way, which connects it quite naturally to the diagrammatics of field theory.

The summation in (17) can be written more explicitly as

\[
\sum_{m=0}^{\infty} \frac{1}{m!} \left( -\frac{\delta I[\eta]}{g} \right)^m = 1 + \sum_{m=1}^{\infty} \frac{(-1)^m}{g^m m!} \prod_{j=1}^{m} \left[ \sum_{n_j=3}^{\infty} \frac{1}{n_j!} \int_0^{\Theta} d\theta_j U^{(n_j)}[q_c(\theta_j)] \eta^{n_j}(\theta_j) \right].
\]

(35)

As a consequence, one is led to compute integrals of the following type:

\[
\langle \eta(\theta_1) \cdots \eta(\theta_k) \rangle \equiv \int_{\eta(0)=0}^{\eta(\Theta)=0} [D\eta(\theta)] e^{-\frac{1}{g} \left\{ I_2[0,\Theta;\eta] - \int_0^{\Theta} d\theta J(\theta) \eta(\theta) \right\}}.
\]

(36)

Such integrals emerge naturally as functional derivatives of the following generating functional:

\[
Z[J] = \int_{\eta(0)=0}^{\eta(\Theta)=0} [D\eta(\theta)] e^{-\frac{1}{g} \left\{ I_2[0,\Theta;\eta] - \int_0^{\Theta} d\theta J(\theta) \eta(\theta) \right\}}.
\]

(37)

Indeed,

\[
\langle \eta(\theta_1) \cdots \eta(\theta_k) \rangle = g^k \frac{\delta^k Z[J]}{\delta J(\theta_1) \cdots \delta J(\theta_k)} \bigg|_{J=0}.
\]

(38)

In order to compute \(Z[J]\), we define

\[
\eta(\theta) = \tilde{\eta}(\theta) + \int_0^{\Theta} d\theta' \mathcal{G}(\theta, \theta') J(\theta'),
\]

(39)

where \(\tilde{\eta}(0) = \tilde{\eta}(\Theta) = 0\), and \(\mathcal{G}(\theta, \theta')\) satisfies

\[
\left\{ -\frac{\partial^2}{\partial \theta^2} + U''[q_c(\theta)] \right\} \mathcal{G}(\theta, \theta') = \delta(\theta - \theta'), \quad \mathcal{G}(0, \theta') = \mathcal{G}(\Theta, \theta') = 0.
\]

(40)

Inserting (39) in (37), and noting that \([D\eta(\theta)] = [D\tilde{\eta}(\theta)]\), we obtain

\[
Z[J] = e^{\frac{1}{2g} \int_0^{\Theta} d\theta \int_0^{\Theta} d\theta' J(\theta) \mathcal{G}(\theta, \theta') J(\theta')} \int_{\tilde{\eta}(0)=0}^{\tilde{\eta}(\Theta)=0} [D\tilde{\eta}(\theta)] e^{-I_2[0,\Theta;\tilde{\eta}]}/g.
\]

(41)

The path integral in (41) has the same form as the one in (20), so we finally arrive at

\[
Z[J] = G_c(0,0;\Theta,0) \exp \left[ \frac{1}{2g} \int_0^{\Theta} d\theta \int_0^{\Theta} d\theta' J(\theta) \mathcal{G}(\theta, \theta') J(\theta') \right].
\]

(42)

Using this result, we can now calculate (38). The result is simply

\[
\langle \eta(\theta_1) \cdots \eta(\theta_k) \rangle = g^{k/2} G_c(0,0;\Theta,0) \sum_P \mathcal{G}(\theta_{i_1}, \theta_{i_2}) \cdots \mathcal{G}(\theta_{i_{k-1}}, \theta_{i_k}),\]

(43)
if \( k \) is even, and zero otherwise. \( \sum_P \) denotes sum over all possible pairings of the \( \theta_i, j \). Inserting this into (17) and (35) yields the semiclassical series for \( Z(\Theta) \).

We still have to solve Eq. (40). This can be easily done if one notes that, for \( \theta \neq \theta' \), it has the same form as Eq. (22). Therefore, \( G(\theta, \theta') \) can be constructed, just as \( \eta_e(\theta) \) itself, as a linear combination of the \( \eta_a(\theta) \) and \( \eta_b(\theta) \) defined previously:

\[
G(\theta, \theta') = \begin{cases} 
  a - \eta_a(\theta) + b - \eta_b(\theta), & \theta < \theta' \\
  a + \eta_a(\theta) + b + \eta_b(\theta), & \theta > \theta'. 
\end{cases}
\]

(44)

Continuity imposes

\[
G(\theta' + \epsilon, \theta') = G(\theta' - \epsilon, \theta'),
\]

whereas (40) leads to

\[
\left. \frac{\partial}{\partial \theta} G(\theta, \theta') \right|_{\theta = \theta' + \epsilon} - \left. \frac{\partial}{\partial \theta} G(\theta, \theta') \right|_{\theta = \theta' - \epsilon} = -1,
\]

(46)

with \( \epsilon \to 0^+ \). (45), (46) and the boundary conditions completely determine the coefficients in (44). The final result is

\[
G(\theta, \theta') = \frac{\Omega(0, \theta < \Theta) \Omega(\theta > \Theta)}{\Omega(0, \Theta)},
\]

(47)

where \( \theta < (\theta >) \equiv \min(\max)\{\theta, \theta'\} \), and \( \Omega(\theta_1, \theta_2) \) is the function defined in (26).

**III. THE SINGLE-WELL QUARTIC OSCILLATOR**

In this section, we study the potential

\[
V(x) = \frac{1}{2} m \omega^2 x^2 + \frac{1}{4} \lambda x^4.
\]

(48)

Choosing \( \omega_N = \omega \) and \( x_N = \sqrt{m \omega^2 / \lambda} \), and introducing the dimensionless quantities of section II, we have \( g = \lambda \hbar / m^2 \omega^3 \) and

\[
U(q) = \frac{1}{2} q^2 + \frac{1}{4} q^4.
\]

(49)

Integrating (11) leads to (10, 11)

\[
q_c(\theta) = q_1 \text{nc}(u_\theta, k),
\]

(50)

where \( \text{nc}(u, k) \equiv 1 / \text{cn}(u, k) \) is one of the Jacobian Elliptic functions (40, 12), and

\[
u_\theta = \sqrt{1 + q_1^2 \left( \theta - \frac{\Theta}{2} \right)}, \quad k = \frac{\sqrt{2 + q_1^2}}{2 (1 + q_1^2)}.
\]

(51)
For future use, we note that (51) can be rewritten as
\[ u_\theta = \frac{2\theta - \Theta}{2\sqrt{2k^2 - 1}}, \quad |q_t| = \sqrt{\frac{2(1 - k^2)}{2k^2 - 1}}. \] (52)

The relation between \( q_0 \) and \( q_t \) is obtained by taking \( \theta = \Theta \) in (50):
\[ q_0 = q_c(\Theta) = q_t \text{ nc } u_\theta. \] (53)

(We shall often omit the \( k \)-dependence in the Jacobian Elliptic functions.)

The action for the classical path (50) is
\[ I[q_c] = \Theta U(q_t) + \sqrt{2} \int_{|q_0|}^{|q_t|} dq \sqrt{(q^2 + q_t^2 + 2)(q^2 - q_t^2)}. \] (54)

Performing the integral [Ref. [40], formula 3.155.6] and replacing \( q_0 \) by the r.h.s. of (53), we obtain
\[ I[q_c] = \Theta \left( \frac{1}{2} q_t^2 + \frac{1}{4} q_t^4 \right) + \frac{4}{3} \left\{ -\sqrt{1 - q_t^2} \left[ E(\varphi_\theta, k) + \frac{1}{2} q_t^2 u_\theta \right] \right. \\
+ \text{sn } u_\theta \left( 1 + \frac{1}{2} q_t^2 \text{ nc }^2 u_\theta \right) \sqrt{1 + \frac{1}{2} q_t^2 \left( 1 + \text{nc }^2 u_\theta \right)} \right\}, \] (55)

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

For the construction of the quadratic semiclassical propagator we shall need
\[ \eta_a(\theta) = \dot{q}_c(\theta) = q_t \sqrt{1 + q_t^2 \text{ sn } u_\theta \text{ dn } u_\theta \text{ nc }^2 u_\theta}, \] (56)
and
\[ Q(\theta) = q_t^{-2}(1 + q_t^2)^{-3/2} \left[ \left( 1 - \frac{1}{k^2} \right) u_\theta + \left( \frac{1}{k^2} - 2 \right) E(\varphi_\theta, k) \right. \]
\[ - \frac{\text{cn } u_\theta \text{ dn } u_\theta}{\text{sn } u_\theta} + \left( k^2 - 1 \right) \frac{\text{cn } u_\theta \text{ sn } u_\theta}{\text{dn } u_\theta} \right]. \] (57)

We may then obtain \( \eta_b(\theta) = \dot{q}_c(\theta) Q(\theta) \) and, thus, \( \Omega_{12} \) and \( W_{12} \) from (29) and (30). Finally, use of (32) will yield the desired propagator.

For the series expansion of the partition function (18), we shall need
\[ \delta U(\theta, \eta) = q_c(\theta) \eta^3 + \frac{1}{4} \eta^4, \] (58)

obtained from (16). Therefore, we have to consider not only the usual quartic vertex, but an additional time(\( \theta \))-dependent cubic term. This completes the set of ingredients needed to write down a semiclassical series for any correlation. In the next subsection, we shall concentrate on the first term of the series (18) for \( Z(\Theta) \), which yields the quadratic approximation.
A. The quadratic approximation for $Z(\Theta)$

From the knowledge of the classical action and of the Van Vleck determinant, we define

$$Z_2(\Theta) \equiv \int_{-\infty}^{\infty} dq_0 \ e^{-i[q_0]/g} \Delta^{-1/2}$$

(59)

as the quadratic approximation to $Z(\Theta)$. To perform the integral over $q_0$ one must write $I[q_c]$ and $\Delta$ solely in terms of $q_0$ (and $\Theta$), but except in rare cases this is not an easy task. Usually, it is much simpler to write these quantities in terms of $q_t$ [see Eq. (53) and Appendix C], and so it is natural to trade $q_0$ for $q_t$ as the integration variable in (59). This is much simplified by the fact that the Jacobian of the map $q_0 \rightarrow q_t$ is simply related to the van Vleck determinant. In fact, Eqs. (12) and (33) imply

$$\left(\frac{\partial q_0}{\partial q_t}\right)_\Theta = -\left(\frac{\partial \Theta}{\partial q_t}\right)_{q_0} = \frac{1}{2} v(q_0, q_t) \left(\frac{\partial \Theta}{\partial q_0}\right)_{q_0} = -\frac{U'(q_t) \Delta}{4\pi g v(q_0, q_t)}.$$  

(60)

Eq. (59) then becomes

$$Z_2(\Theta) = \frac{1}{4\pi g} \int_{q_0^+}^{q_0^-} dq_t \frac{U'(q_t) \Delta^{1/2}}{v(q_0, q_t)} e^{-i[q_0]/g} \equiv \int_{q_0^+}^{q_0^-} dq_t \ D(q_t, \Theta) \ e^{-i[q_0]/g},$$

(61)

where $q_0^\pm \equiv \lim_{q_0 \to \pm\infty} q_t(q_0, \Theta)$.

The expression above is valid for single-well potentials in general. Now, let us especialize to the potential (49). $I[q_c]$ is given by (55), and using (33) and (57) one can write $D(q_t, \Theta)$ as

$$D(q_t, \Theta) = \left(1 + q_t^2\right)^{1/4} \sqrt{4\pi g} \left[1 - k^2 \frac{1}{k^2} u_\Theta + 2k^2 - 1 \ k^2 E(\varphi_\Theta, k) + \frac{cn u_\Theta dn u_\Theta}{sn u_\Theta} + (1 - k^2) \ \frac{cn u_\Theta sn u_\Theta}{dn u_\Theta}\right]^{1/2}.$$  

(62)

From (53) it follows that $q_0 \rightarrow \infty$ when $cn(u_\Theta, k) = 0$, which occurs when $u_\Theta = K(k)$, where $K(k)$ is the Complete Elliptic Integral of the First Kind. Using (52), this condition can be written as an equation in $k$:

$$\frac{\Theta}{2\sqrt{2k^2 - 1}} = K(k).$$  

(63)

The graph of $f(k) \equiv 2\sqrt{2k^2 - 1} K(k)$ is plotted in Fig. 2. It increases monotonically from zero (at $k = 1/\sqrt{2}$) to infinity (as $k \rightarrow 1$), and so for each nonnegative value of $\Theta$ Eq. (53) has a unique solution, which we denote by $k_\Theta$. Eq. (52) then gives the corresponding value of $q_{\Theta}^\pm$ ($q_{\Theta}^- = -q_{\Theta}^+$, since $U(-q) = U(q)$).

B. Limiting cases of the quadratic approximation

Expression (61) may be used to compute $Z_2(\Theta)$ numerically for any value of $\Theta$. However, certain limiting cases may be dealt with analytically, and it is instructive to consider them first in order to recover some known results, thus providing a consistency check. These limits are: (1) the harmonic oscillator ($g \rightarrow 0$), (2) high temperatures ($\Theta \rightarrow 0$), and (3) low temperatures ($\Theta \rightarrow \infty$).
1. The harmonic oscillator

Since \( V(x) = \frac{1}{2} m \omega^2 x^2 \) when \( g = 0 \), one should obtain the partition function of the harmonic oscillator in the limit \( g \to 0 \). To see how to arrive at this result starting from the expressions derived in this section, we note that in this limit one can perform the integral (61) using the steepest descent method. For this, we only need the first nontrivial term in the series expansion of \( I[q_c] \) and \( D(q_t, \Theta) \) around \( q_t = 0 \).

When \( |q_t| \ll 1 \), one has \( k \approx 1 - \frac{1}{4} q^2_t \) and \( k'^2 \equiv 1 - k^2 \approx \frac{1}{2} q^2_t \ll 1 \). Now, we use the smallness of \( k' \) to derive an approximation for \( E(\varphi_\Theta, k) \). The first step is to write it in terms of \( k' \):

\[
E(\varphi, k) = \int_0^\varphi \sqrt{1 - k'^2} \sin x\, dx = \int_0^\varphi \cos x \sqrt{1 + k'^2 \tan^2 x}\, dx.
\]  
(64)

Expanding the integrand to first order in \( k'^2 \), integrating the result, and using the fact that \( \sin \varphi_\Theta = \text{sn} u_\Theta \) and \( \cos \varphi_\Theta = \text{cn} u_\Theta \), we finally obtain

\[
E(\varphi_\Theta, k) \approx \text{sn} u_\Theta + \frac{1}{4} q^2_t \left[ \ln \left( \frac{1 + \text{sn} u_\Theta}{\text{cn} u_\Theta} \right) - \text{sn} u_\Theta \right].
\]  
(65)

Inserting this result in (55) and expanding the square-roots in that equation in powers of \( q_t \), one obtains

\[
I[q_c] = q^2_t \left[ \frac{1}{2} \Theta - \frac{2}{3} u_\Theta - \frac{1}{3} \ln \left( \frac{1 + \text{sn} u_\Theta}{\text{cn} u_\Theta} \right) + \text{sn} u_\Theta \text{nc}^2 u_\Theta \right] + O(q^4_t).
\]  
(66)

Now, we use the fact that \( u_\Theta \to \Theta/2 \) and \( k \to 1 \) when \( q_t \to 0 \), and \( \text{sn}(u, 1) = \tanh u \) and \( \text{cn}(u, 1) = \text{sech} u \), thus finally arriving at

\[
I[q_c] = \frac{1}{2} q^2_t \sinh \Theta + O(q^4_t).
\]  
(67)

In the case of \( D(q_t, \Theta) \) it is enough to take the limit \( q_t \to 0 \) in (52). Then, the first and the last term in square brackets vanish, the second approaches \( \tanh(\Theta/2) \) [use (53)], and the third approaches \( \text{sech}^2(\Theta/2) \coth(\Theta/2) \). Combining these results, one obtains

\[
D(q_t, \Theta) = [4\pi g \tanh(\Theta/2)]^{-1/2} + O(q^2_t).
\]  
(68)

Inserting (57) and (58) in (61) yields the desired small-\( g \) limit of the partition function:

\[
Z_2(\Theta) \stackrel{g \to 0}{\sim} \int_{-\infty}^{\infty} e^{-\left(1/2g\right) q^2_t \sinh \Theta} dq_t = \frac{1}{2 \sinh(\Theta/2)}.
\]  
(69)
2. High temperatures

At high temperatures, $\Theta \to 0$ and (63) is solved for $k_\Theta \to 1/\sqrt{2}$, and so $q_0^+ \to \infty$. To lowest order in $\Theta$, one has $\text{cn} \ u_\Theta \approx \text{nc} \ u_\Theta \approx \text{dn} \ u_\Theta \approx 1$, $\text{sn} \ u_\Theta \approx u_\Theta$ and $E(\varphi_\Theta, k) \approx \varphi_\Theta \approx u_\Theta$, and so the term in curly brackets in (55) vanishes in order $\Theta$:

$$I[q_e] = \Theta U(q_e) + \mathcal{O}(\Theta^2).$$

(70)

In $D(q_\ell, \Theta)$, Eq. (62), the third term in square brackets behaves as $u_\Theta^{-1}$, while all the others behave as $u_\Theta$ when $\Theta \to 0$. One has, therefore,

$$D(q_\ell, \Theta) = (2\pi g \Theta)^{-1/2} + \mathcal{O}(\Theta^{3/2}).$$

(71)

It follows that

$$Z_2(\Theta) \sim \theta \sqrt{\frac{1}{2\pi g \Theta}} \int_{-\infty}^{\infty} dq \ e^{-\Theta U(q)/g},$$

(72)

or, equivalently,

$$Z_2(\beta) \sim \sqrt{\frac{m}{2\pi \hbar^2 \beta}} \int_{-\infty}^{\infty} dx \ e^{-\beta V(x)},$$

(73)

with $V(x)$ and $U(q)$ defined in (48) and (49). This is, clearly, the “classical” limit for the partition function with a pre-factor that incorporates quantum fluctuations.

3. Low temperatures

At low temperatures, $\Theta \to \infty$ and (63) is solved for $k_\Theta \to 1$. Using the asymptotic expansion [Ref. [10], formula 8.113.1]

$$K(k) = \ln (4/k') + \frac{1}{4} \left[ \ln (4/k') - 1 \right] k'^2 + \cdots,$$

(74)

valid for $k' \equiv \sqrt{1 - k^2} \to 0$, it follows from (63) that $k'_\Theta \approx 4 e^{-\Theta/2}$ in leading order. Therefore,

$$q_0^+ = \sqrt{\frac{2k'^2_\Theta}{1 - 2k'^2_\Theta}} \approx 4 \sqrt{2} e^{-\Theta/2}.$$

(75)

Since $|q_t| \leq q_0^+ \ll 1$, one has $k \approx 1$, $u_\Theta \approx \Theta/2$ and $E(\varphi_\Theta, k) \approx \text{sn}(u_\Theta, k) \approx \tanh(\Theta/2) \approx 1$ in the whole range of integration. One can also neglect $\Theta U(q_t)$ and $q_t^2 u_\Theta$ in (55), since both terms behave as $\Theta e^{-\Theta}$. However, one must be more careful with the combination $q_t^2 \text{nc}^2 u_\Theta (= q_0^2)$, since it grows very rapidly with $q_t$ (in fact diverging when $|q_t| \to q_0^+$), and so cannot be treated as a formally small quantity.

Leaving this combination “untouched” in (55), but making use of the approximations listed above, we obtain
\[ I[q_c] = \frac{4}{3} \left[ \left(1 + \frac{1}{2} q_t^2 u_\Theta \right)^{3/2} - 1 \right] + \mathcal{O} \left( \Theta e^{-\Theta} \right). \tag{76} \]

The analysis of \( D(q_t, \Theta) \) is much simpler. One can simply take the limit \( \Theta \to \infty \) of (68), which was derived under the assumption that \( q_t \ll 1 \).

Putting all pieces together we finally obtain

\[ Z_2(\Theta) \sim \int_{-q_0^+}^{q_0^+} dq_t \sqrt{4\pi g} e^{-I[q_c]/g}, \tag{77} \]

with \( q_0^+ \) and \( I[q_c] \) given by (75) and (76), respectively.

**C. Applications**

We shall now apply the quadratic semiclassical approximation to obtain the ground-state energy and the curve for the specific heat as a function of temperature. These two applications will teach us about the usefulness of the approximation.

In order to compare (77) with the expected low-temperature limit of the partition function, \( Z(\Theta) \sim e^{-\Theta \varepsilon_0(g)} \) (where \( \varepsilon_0(g) \equiv E_0(g)/\hbar \omega \) is the dimensionless ground state energy), it is convenient to rewrite it in a form in which the \( \Theta \)-dependence can be analyzed more easily. This can be done by changing the integration variable back to \( q_0 \). Since \( q_t nc u_\Theta = q_0 \) and \( q_0^+ \) is the value of \( q_t \) corresponding to \( q_0 \to \infty \), one has

\[ Z_2(\Theta) \sim \int_{-\infty}^{\infty} dq_0 \sqrt{\frac{\partial q_t}{\partial q_0}} \exp \left\{ -\frac{4}{3g} \left[ \left(1 + \frac{1}{2} q_0^2 \right)^{3/2} - 1 \right] \right\}. \tag{78} \]

When \( \Theta \gg 1 \) it is possible to write an approximate expression for \( q_t(q_0, \Theta) \), thus allowing to write the integrand in (78) solely in terms of \( q_0 \) and \( \Theta \). The final result is (see Appendix D for details)

\[ Z_2(\Theta) \sim 2 e^{-\Theta/2} \sqrt{\frac{\pi g}{\varepsilon_0^2}} \int_{-\infty}^{\infty} dq_0 \frac{\exp \left\{ -\frac{4}{3g} \left[ \left(1 + \frac{1}{2} q_0^2 \right)^{3/2} - 1 \right] \right\}}{\sqrt{1 + \frac{1}{2} q_0^2 \left(1 + \sqrt{1 + \frac{1}{2} q_0^2} \right)}}. \tag{79} \]

This gives \( \varepsilon_0(g) = 1/2 \), indicating that the quadratic approximation is insufficient to yield corrections to the ground state energy of the harmonic oscillator. On the other hand, if one recalls that the partition function can be written as

\[ Z(\Theta) = \int_{-\infty}^{\infty} \rho(\Theta; q, q) dq, \tag{80} \]

where

\[ \rho(\Theta; q, q) = \sum_n e^{-\Theta \varepsilon_n} |\psi_n(q)|^2 \sim \int_{-\infty}^{\infty} dq_0 \rho(\Theta; q_0, q) \tag{81} \]

is the diagonal element of the density matrix, one may take the square root of the integrand in (79) as an approximation to the (unnormalized) wave function of the ground state. To
test the accuracy of this approximation, we have evaluated the expectation values of the energy for some values of $g$ and compared them with high precision results found in the literature. As Table I shows, the ground state energy computed with this “semiclassical” wave function differs from the exact one by less than 1% even for $g$ as large as 2.

Another concrete problem that can be treated is the calculation of the specific heat of the quantum anharmonic oscillator. It can be written in terms of $Z(\Theta)$ as

$$C = \Theta^2 \left[ \frac{1}{Z} \frac{\partial^2 Z}{\partial \Theta^2} - \left( \frac{1}{Z} \frac{\partial Z}{\partial \Theta} \right)^2 \right]. \quad (82)$$

This expression was computed using MAPLE for a few values of $\Theta$ and the coupling constant value $g = 0.3$. The result is depicted in Fig. 3, which also exhibits the curve of specific heat of the classical anharmonic oscillator (solid line). As expected, the results agree when the temperature is sufficiently high, but, in contrast to the classical result, the semiclassical approximation is qualitatively correct at low temperatures too, dropping to zero as $T \to 0$.

This result, together with the estimate for the ground-state obtained previously, shows that the quadratic approximation works very well, being quite accurate at high temperatures, and still reliable at lower temperatures. In the next subsection, we will comment on why this is so.

**D. Beyond quadratic**

In this subsection, we shall compute the first correction $G_1$ to the quadratic approximation. For the sake of comparison, we shall use both the quantum-mechanical (section II.A) and the field theory approaches (section II.B).

In the quantum-mechanical approach, we want to compute

$$G_1(q_0, \Theta) = \int_0^\Theta d\theta \int_{-\infty}^\infty d\eta G_c(0,0;\theta,\eta) \delta U[\theta,\eta] G_c(\theta,\eta;\Theta,0), \quad (83)$$

with $\delta U$ given by (58), and $G_c$ constructed from (56) and (57), using (29) and (30). Since $G_c$ is gaussian in $\eta$, and $\delta U$ is a polynomial in $\eta$, the integral in $\eta$ can be readily performed, yielding

$$G_1(q_0, \Theta) = \frac{3}{4} g^2 \left[ \frac{1}{\sqrt{4\pi g q_c^2(0)} Q(0)} \right] \int_0^\Theta d\theta \frac{\dot{q}_c^4(\theta) [Q^2(\theta) - Q^2(0)]^2}{4Q^2(0)}, \quad (84)$$

where the bracket in front can be identified with $G_c(0,0;\Theta,0)$.

In the field-theoretic approach, we arrive at the same expression. In fact, the first correction corresponds to the $m = 1$ term in (17) which, using (28), yields

$$G_1(q_0, \Theta) = \int_0^\Theta d\theta \left[ q_c(\theta) \langle \eta^3(\theta) \rangle + \frac{1}{4} \langle \eta^4(\theta) \rangle \right]. \quad (85)$$

Using (43), we obtain
\[
G_1(q_0, \Theta) = \frac{3}{4} g^2 G_c(0, 0; \Theta, 0) \int_0^\Theta d\theta G^2(\theta, \theta). \tag{86}
\]

\((\langle \eta^3 \rangle\text{ vanishes, and the factor 3 comes from the three possible pairings of the four } \eta\text{'s in } \langle \eta^4 \rangle\text{.) Using (47) and (29) we reobtain (84).}

Inserting (86) in (61) and changing the integration variable from \(q_0\) to \(q_t\) gives
\[
Z(\Theta) = \int_{q_t^0}^{q_t^+} dq_t D(q_t; \Theta) e^{-I[q_c]/g} \left[ 1 - ga_1(q_t, \Theta) + \ldots \right], \tag{87}
\]
where
\[
a_1(q_t, \Theta) = \frac{3}{4} \int_0^{\Theta} d\theta G^2(\theta, \theta). \tag{88}
\]

Because of the complicated form of \(G(\theta, \theta)\), it is not a simple task to compute \(a_1(q_t, \Theta)\). However, we can estimate the magnitude of this term without much effort. Indeed, as shown in Appendix \ref{sec:appE}, \(G(\theta, \theta)\) obeys the following inequality:

\[
G(\theta, \theta) \leq \frac{\Theta(\Theta - \theta)}{\Theta} \quad (0 \leq \theta \leq \Theta). \tag{89}
\]

Therefore,
\[
a_1(q_t, \Theta) \leq \frac{\Theta^3}{40}. \tag{90}
\]

This shows that (in the case of the quartic anharmonic oscillator) the quadratic approximation to the partition function, Eq. (59) or (61), can be used with confidence whenever the condition \(g\Theta^3/40 \ll 1\) is satisfied; this accounts for the numerical agreements obtained in the applications of the quadratic approximation.

A last comment is in order: the next term in the expansion for \(Z(\Theta)\) has a piece with a factor \(g\) and one with a factor \(g^2\). The former comes from the product of \(\langle \eta^6 \rangle \sim g^3\) with the overall \(g^{-2}\), whereas the latter involves \(\langle \eta^8 \rangle \sim g^4\). This is another indication that we are not dealing with a perturbative series.

\section*{IV. CONCLUSIONS}

In order to understand the nature of the semiclassical series for the partition function, it is instructive to look at a diagrammatic expansion of \(\rho(\Theta; q, q)\), which appears in (50). Comparing with (18), and defining \(\rho_c(\theta_1, \eta_1; \theta_2, \eta_2) \equiv e^{-I[\theta_1, \theta_2; q_c]/g} G_c(\theta_1, \eta_1; \theta_2, \eta_2)\), we have the expansion in Fig. 4, where the dot represents the point \(q\), the squares stand for the insertions of \([(-1)g^{-1}\delta U]\), the dashed lines for \(\rho_c\), while the full line represents \(\rho(\Theta, q, q)\). From (20) and (21), we may expand \(\rho_c\) itself in terms of the density matrix elements for the harmonic oscillator (add and subtract 1 to \(U''[q_c]\) in (21)), to obtain Fig. 3, where the circles represent insertions of \([(-1)g^{-1}[U''[q_c] - 1]]\), and the dotted lines stand for the density matrix elements of the harmonic oscillator. Therefore, even the first term in our series already corresponds to an infinite sum of perturbative diagrams. Analogously, one could use
the Feynman diagrams of the field-theoretic description to arrive at the same conclusion. This is a clear indication of the nonperturbative nature of our treatment.

The results of section II can be generalized to higher-dimensional Quantum Statistical Mechanics, just as in Quantum Mechanics, where this was accomplished in [26,27]. The generalization to potentials which allow for more than one classical solution, such as the double-well quartic anharmonic oscillator, requires a subtle matching of the series around each appropriate saddle-point (i.e., the minima). This is presently under investigation [28].

An extension of our results to field theories is hampered by the fact that we do not know how to construct a semiclassical propagator in general. The technical simplifications which appear in one dimension cease to exist. However, our methods may still be of use in problems where classical solutions have a lot of symmetry (e.g., spherical symmetry) so that we can reduce them to effective one-dimensional problems. There are many such examples in Physics: instantons, monopoles, vortices and solitons are a few of the backgrounds that fall into that category. It is our intention to pursue this line of investigation.

Finally, we should remark that the field-theoretic treatment of subsection II B can be used to compute any correlation function of interest. Therefore, a semiclassical series can be written down for any physical quantity once it is expressed in terms of the relevant correlations.

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APPENDIX A:

Here we show that \( \eta_b(\theta) \), as defined in subsection II A, is continuous at \( \theta = \Theta/2 \), and that it is also possible to make \( \dot{\eta}_b(\theta) \) continuous there by a suitable choice of \( Q(0) \).

To prove that \( \eta_b(\theta) \) is continuous at \( \Theta/2 \), we have to show that the limits \( \lim_{\theta \to \Theta/2} \eta_b(\theta) \) and \( \lim_{\theta \to \Theta/2} \dot{\eta}_b(\theta) \) exist and are equal. However, since \( \eta_b(\theta) \) is even with respect to reflection around \( \Theta/2 \), it suffices to prove the existence of one of them; the existence of the other and their equality will then be automatically satisfied. Thus, let us consider the former limit:

\[
\lim_{\theta \to \Theta/2} \eta_b(\theta) = \lim_{\theta \to \Theta/2} \left[ Q(0) \dot{q}_c(\theta) + \dot{q}_c(\theta) \int_0^\theta \frac{d\theta'}{q_c^2(\theta')} \right] = 0 + \lim_{q_0 \to q_t} v(q,q_t) \int_{q_0}^q \frac{dq'}{v^3(q',q_t)}. \quad (A1)
\]

To compute the above limit, we divide the interval of integration in two subintervals, \([q_0, \bar{q}]\) and \([\bar{q}, q]\), with \( \bar{q} \) close to \( q_t \) but fixed. Then \( v(q,q_t) \) times the first integral vanishes when \( q \to q_t \) and, by expanding \( U(q) \) around \( q_t \), we can approximate \( v(q,q_t) \) times the second integral by
\[
\sqrt{2 U'(q_t)(q - q_t)} \int_q^{q_t} \frac{dq'}{[2 U'(q_t)(q' - q_t)]^{3/2}}.
\]

(A2)

Computing the integral and taking the limit, we finally obtain

\[
\lim_{\theta \uparrow \Theta/2} \eta_b(\theta) = -\frac{1}{U'(q_t)}.
\]

(A3)

Let us now compute the limit

\[
\lim_{\theta \uparrow \Theta/2} \dot{\eta}_b(\theta) = \lim_{\theta \uparrow \Theta/2} \left[ Q(0) \ddot{q}_c(\theta) + \ddot{q}_c(\theta) \int_0^\theta \frac{d\theta'}{\dot{q}_c^2(\theta')} + \frac{1}{\dot{q}_c(\theta)} \right].
\]

(A4)

Using (10) and (11), and an integration by parts that cancels divergences, yields

\[
\lim_{\theta \uparrow \Theta/2} \dot{\eta}_b(\theta) = U'(q_t) \left[ Q(0) + \frac{1}{U'(q_0)v(q_0, q_t)} - \int_{q_0}^{q_t} \frac{U''(q) dq}{[U'(q)]^2 v(q, q_t)} \right].
\]

(A5)

(Although the integrand in the integrand in (A5) is singular as \( q \to q_t \), the singularity is integrable.) Using (12) we may rewrite (A5) as

\[
\lim_{\theta \uparrow \Theta/2} \dot{\eta}_b(\theta) = Q(0) U'(q_t) + \frac{1}{2} \left( \frac{\partial \Theta}{\partial q_t} \right)_{q_0}.
\]

(A6)

Applying the limit \( \dot{\eta}_b(\theta) \) is odd with respect to reflection around \( \Theta/2 \), \( \lim_{\theta \downarrow \Theta/2} \dot{\eta}_b(\theta) = -\lim_{\theta \uparrow \Theta/2} \dot{\eta}_b(\theta) \). However, for \( \dot{\eta}_b(\theta) \) to be continuous at \( \Theta/2 \), those limits must be equal. This is possible only if \( \lim_{\theta \uparrow \Theta/2} \dot{\eta}_b(\theta) = 0 \), or

\[
Q(0) = -\frac{1}{U'(q_t)} \left( \frac{\partial \Theta}{\partial q_t} \right)_{q_0}.
\]

(A7)

APPENDIX B:

In this appendix, we compute the pre-factor in (23). To do so, we remark that (20) is the path-integral expression for the Euclidean time evolution operator \( \hat{\rho}_c \) of the quantum-mechanical time-dependent problem defined by (note that the role of \( \hbar \) is played by \( g \) )

\[
-g \frac{\partial}{\partial \theta} \hat{\rho}_c(\theta, \theta') = \hat{H}_c(\theta) \hat{\rho}_c(\theta, \theta'),
\]

(B1)

with

\[
\hat{H}_c(\theta) = -\frac{g^2}{2} \frac{\partial^2}{\partial q^2} + \frac{1}{2} U''[q_c(\theta)] q^2.
\]

(B2)

Indeed, we have

\[
G_c(\theta_1, \eta_1; \theta_2, \eta_2) = \langle \eta_2 | \hat{\rho}_c(\theta_2, \theta_1) | \eta_1 \rangle,
\]

(B3)
so that \( G_c(\theta_1, \eta_1; \theta_2, \eta_2) \) is a density matrix element.

Inserting (23) into (B1), and using the fact that \( I_2 \) satisfies the Hamilton-Jacobi equation

\[
\frac{\partial I_2}{\partial \theta_2} + \frac{1}{2} \left( \frac{\partial I_2}{\partial \eta_2} \right)^2 - \frac{1}{2} U''(q_c(\theta_2)) \eta_2^2 = 0,
\]

(B4)

leads to

\[
\left( \frac{\partial}{\partial \theta_2} + \frac{1}{2} \frac{W_{12}}{\Omega_{12}} \right) G_c(\theta_1, 0; \theta_2, 0) = 0,
\]

(B5)

whose solution is (note that \( W_{12} = \partial \Omega_{12} / \partial \theta_2 \))

\[
G_c(\theta_1, 0; \theta_2, 0) = C(\theta_1) \Omega_{12}^{-1/2}.
\]

(B6)

\( C(\theta_1) \) can be determined by demanding that we recover the free-particle result as \( \theta_1 \to \theta_2 \),

\[
G_c(\theta_1, 0; \theta_2, 0) \mid_{\theta_1 \to \theta_2} = \left[ 2\pi g (\theta_2 - \theta_1) \right]^{-1/2}.
\]

(B7)

Expanding \( \Omega_{12} \) around \( \theta_1 \), we obtain

\[
\Omega_{12} = \Omega_{11} + \left. \frac{\partial \Omega_{12}}{\partial \theta_2} \right|_{\theta_2 = \theta_1} (\theta_2 - \theta_1) + \ldots = W_{11} (\theta_2 - \theta_1) + \ldots
\]

(B8)

Inserting this result in (B6) and comparing with (B7) we finally obtain

\[
G_c(\theta_1, 0; \theta_2, 0) = \left[ \frac{W_{11}}{2\pi g \Omega_{12}} \right]^{1/2}.
\]

(B9)

**APPENDIX C:**

Here we provide a simple argument to show why it is usually simpler to write \( q_0(q_t, \Theta) \) rather than \( q_t(q_0, \Theta) \). In fact, using \( \zeta = q/q_t \) as integration variable in Eq. (12), one has

\[
\Theta = \int_{q_t}^{q_0/q_t} \frac{2|q_t| d\zeta}{\sqrt{2[U(\zeta q_t) - U(q_t)]}} = F_{q_t}(q_0/q_t) - F_{q_t}(1),
\]

(C1)

where \( F_{q_t}(\zeta) \) denotes the primitive of \( 2|q_t|/\sqrt{2[U(\zeta q_t) - U(q_t)]} \). One can then solve (C1) for \( q_0 \), thus obtaining

\[
q_0 = q_t F_{q_t}^{-1}[\Theta + F_{q_t}(1)].
\]

(C2)
APPENDIX D:

In this appendix, we derive an approximate expression for \( q_t(q_0, \Theta) \) valid for \( \Theta \gg 1 \). We start by writing (12) with \( U(q) \) given by (49):

\[
\Theta = 2 \sqrt{2} \left( \int_{|q_t|}^a dq \frac{d}{\sqrt{(q^2 - q_t^2)(q^2 + q_t^2 + 2)}} \right) \equiv I_1 + I_2, \quad (D1)
\]

where \( a \) is a positive number such that \( 1 \gg a \gg |q_t| \) (that both inequalities can be simultaneously satisfied is guaranteed by the fact that \( |q_t| \leq q_0^+ \approx 4 \sqrt{2} e^{-\Theta/2} \) when \( \Theta \gg 1 \)). Now, since both \( a \) and \( |q_0| \) are much greater than \( |q_t| \) to write

\[
I_1 \approx 2 \int_{|q_t|}^a dq \frac{d}{\sqrt{q^2 - q_t^2}} = 2 \cosh^{-1} \left( \frac{a}{|q_t|} \right) \approx 2 \ln \left( \frac{2a}{|q_t|} \right), \quad (D2)
\]

where the last (approximate) equality follows from \( a/|q_t| \) being much greater than 1.

In order to evaluate \( I_2 \), we use the fact that both \( a \) and \( |q_0| \) are much greater than \( |q_t| \) to write

\[
I_2 \approx 2 \sqrt{2} \int_{|q_t|}^{q_0} dq \frac{d}{\sqrt{q^2(q^2 + 2)}} = 2 \ln \left( \frac{|q_0|}{a} \frac{1 + \sqrt{1 + \frac{1}{2} a^2}}{1 + \sqrt{1 + \frac{1}{2} q_0^2}} \right) \approx 2 \ln \left( \frac{2 |q_0| / a}{1 + \sqrt{1 + \frac{1}{2} q_0^2}} \right). \quad (D3)
\]

When adding the above results for \( I_1 \) and \( I_2 \), the dependence on \( a \) cancels out (as it should), and we are left with the following result:

\[
\Theta \approx 2 \ln \left( \frac{4 q_0 / q_t}{1 + \sqrt{1 + \frac{1}{2} q_0^2}} \right). \quad (D4)
\]

This can be solved for \( q_t \), yielding

\[
q_t(q_0, \Theta) \approx \frac{4 q_0 e^{-\Theta/2}}{1 + \sqrt{1 + \frac{1}{2} q_0^2}}. \quad (D5)
\]

Using this expression to calculate the Jacobian in (78) one finally obtains (79).

APPENDIX E:

Let us define the function \( G_0(\theta, \theta') \) as

\[
G_0(\theta, \theta') = \begin{cases} \frac{\theta (\Theta - \theta')}{\Theta}, & \theta \leq \theta' \\ \frac{\theta' (\Theta - \theta)}{\Theta}, & \theta \geq \theta'. \end{cases} \quad (E1)
\]

This function satisfies an equation similar to Eq. (40):
\[-\frac{\partial^2}{\partial \theta^2} G_0(\theta, \theta') = \delta(\theta - \theta'), \quad G_0(0, \theta') = G_0(\Theta, \theta') = 0. \quad (E2)\]

If we multiply (E3) by \(G_0(\theta, \theta')\) and \((E2)\) by \(G(\theta, \theta')\), subtract one from the other, and integrate the result from \(\theta = 0\) to \(\theta = \Theta\), we obtain

\[G_0(\theta', \theta') - G(\theta', \theta') = \int_0^\Theta d\theta U''[q_c(\theta)] G_0(\theta, \theta') G(\theta, \theta'). \quad (E3)\]

In the case of the quartic anharmonic oscillator, \(U''[q_c(\theta)] = 1 + 3q_c^2(\theta) > 0\) and (consequently) \(G(\theta, \theta') \geq 0\) for \(0 \leq \theta, \theta' \leq \Theta\). Since \(G_0(\theta, \theta')\) is also nonnegative in this interval, Eq. \((E3)\) leads to the inequality (89).
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### TABLE I. Ground state energies for different values of $g$ ($\hbar = m = \omega = 1$).

| $g$ | $E_0$ (semiclassical)$^a$ | $E_0$ (exact)$^b$ | error(%) |
|-----|--------------------------|-------------------|-----------|
| 0.4 | 0.559258                 | 0.559146          | 0.02      |
| 1.2 | 0.639765                 | 0.637992          | 0.28      |
| 2.0 | 0.701429                 | 0.696176          | 0.75      |
| 4.0 | 0.823078                 | 0.803771          | 2.40      |
| 8.0 | 1.011928                 | 0.951568          | 6.34      |

$^a$ $\langle \phi_0 | H | \phi_0 \rangle / \langle \phi_0 | \phi_0 \rangle$, where $\phi_0(q_0)$ is the square root of the integrand in Eq. (79).

$^b$ Values quoted from Ref. [43].
FIGURES

FIG. 1. $U(q)$.

FIG. 2. Graph of $f(k)$.

FIG. 3. Specific heat vs. temperature ($T = 1/\Theta$) for the quantum (diamonds) and classical (solid line) anharmonic oscillator. $g = 0.3$.

FIG. 4. Diagrammatic expansion for $\rho(\Theta; q, q)$.

FIG. 5. Diagrammatic expansion for $\rho_c(\Theta; q_1, q_2)$. 
\[ \circ = \bullet + \circ + \square + \bullet + \cdots \]
\[= + \bullet + \bullet + \ldots\]