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Uniform semiclassical approximation in quantum statistical mechanics*

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Abstract

We present a simple method to deal with caustics in the semiclassical approximation to the partition function of a one-dimensional quantum system. The procedure, which makes use of complex trajectories, is applied to the quartic double-well potential.

1 Introduction

It is well known [1] that the partition function for 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 ($\beta = 1/k_B T$):

$$Z(\beta) = \int dx_0 \, \langle x_0 | e^{-\beta \hat{H}} | x_0 \rangle, \tag{1}$$

$$\langle x_0 | e^{-\beta \hat{H}} | x_0 \rangle = \int_{x(0)=x_0}^{x(\beta\hbar)=x_0} [\mathcal{D}x(\tau)] \, e^{-S[x]/\hbar}, \tag{2}$$

$$S[x] = \int_0^{\beta\hbar} d\tau \left[\frac{1}{2} m \dot{x}^2 + V(x) \right]. \tag{3}$$

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The semiclassical approximation to the density matrix element (2) is given by[1]

$$\langle x_0|e^{-\beta\hat{H}}|x_0\rangle \approx \sum_{k=1}^{N} e^{-S[x_c^k]/\hbar}\,\Delta_k^{-1/2}, \tag{4}$$

where $x_c^k(\tau)$ is a classical trajectory [i.e., it is a solution to the Euler-Lagrange equation, $m\ddot{x} = V'(x)$, subject to the boundary conditions $x(0) = x(\beta\hbar) = x_0$] that *minimizes*[2] (globally or locally) the action $S[x]$, and Δ_k is the determinant of of the fluctuation operator $\hat{F}[x_c^k] \equiv -m\,\partial_\tau^2 + V''[x_c^k]$. (A derivation of this result will be sketched in Section 2.)

In Ref. [2] we have examined, for the sake of simplicity, potentials for which there is only one classical trajectory satisfying the above boundary conditions. In general, however, the number N of such solutions depends on x_0 and β. A problem then occurs when we cross a *caustic* [the frontier between two regions of the (x_0, β)-plane characterized by different values of N]: the r.h.s. of (4) diverges [3]. This divergence, however, is unphysical, being an artifact of the semiclassical approximation. The purpose of this work is to present a simple extension of the semiclassical approximation which circumvents this problem.[3] (Due to limitations of space, here we shall only sketch the method. Details will be given elsewhere.)

2 Improved semiclassical approximation

In order to show how one can improve the semiclassical approximation so as to eliminate the unphysical divergences at the caustics, it is convenient to recall how (4) is derived. Briefly, one has to: (i) expand the action around a minimum $x_c(\tau)$: $S[x_c + \eta] = S[x_c] + S_2 + \delta S$, where $S_2 = \frac{1}{2}\int_0^{\beta\hbar} d\tau\,\eta(\tau)\,\hat{F}[x_c(\tau)]\,\eta(\tau)$ and $\delta S = O(\eta^3)$; (ii) throw away δS; (iii) express $\eta(\tau)$ in terms of the orthonormal modes of $\hat{F}$, i.e., $\eta(\tau) = \sum_{j=0}^{\infty} a_j \varphi_j(\tau)$, where $\hat{F}\varphi_j(\tau) = \lambda_j \varphi_j(\tau)$, $\varphi_j(0) = \varphi_j(\beta\hbar) = 0$; then $S_2 = \frac{1}{2}\sum_{j=0}^{\infty}\lambda_j a_j^2$ and $[\mathcal{D}x(\tau)] = \prod_{j=0}^{\infty} da_j/\sqrt{2\pi\hbar}$. The path integral in (2) has now become a product of Gaussian integrals. Performing the integrations one arrives at the "usual" semiclassical approximation to the density matrix element:

$$\langle x_0|e^{-\beta\hat{H}}|x_0\rangle \approx e^{-S[x_c]/\hbar}\,\Delta^{-1/2}, \tag{5}$$

where $\Delta = \prod_{j=0}^{\infty}\lambda_j = \det\hat{F}$. If there are N minima, one has to add together their contributions, thus obtaining (4).

When we cross a caustic, a classical trajectory $x_c(\tau)$ is created or annihilated. Precisely at this point, the lowest eigenvalue of $\hat{F}[x_c]$ vanishes, thus making the integral $\int_{-\infty}^{\infty} da_0\,\exp(-\lambda_0 a_0^2/2\hbar)$ diverge. This problem can be remedied by

[1]Each term in the sum on the r.h.s. of (4) is in fact the first term of a series. See Ref. [2].
[2]The Euclidean nature of the path integral allows one to discard saddle-points.
[3]Ankerhold *et al.* [4] have discussed the caustics problem near the top of a potential barrier. The present work shows how to deal with the problem everywhere.

retaining fluctuations beyond quadratic in the subspace spanned by φ_0 (the eigenmode of $\hat{F}$ associated with λ_0). As a result of this procedure,[4] we obtain an improved approximation to the density matrix element (2):

$$\langle x_0|e^{-\beta\hat{H}}|x_0\rangle \approx e^{-S[x_{\rm gm}]/\hbar}\,\Delta^{-1/2}\,\mathcal{F}(x_0,\beta), \tag{6}$$

where $x_{\rm gm}(\tau)$ is the *global minimum* of $S[x]$ and

$$\mathcal{F}(x_0,\beta) \equiv \sqrt{\frac{\lambda_0}{2\pi\hbar}}\int_{-\infty}^{\infty} da_0\, e^{-\mathcal{V}(a_0)/\hbar}, \tag{7}$$

with

$$\mathcal{V}(a_0) = \frac{1}{2}\,\lambda_0 a_0^2 + \sum_{n=3}^{M}\left(\int_0^{\beta\hbar} d\tau\, V^{(n)}[x_{\rm gm}(\tau)]\,\varphi_0^n(\tau)\right)\frac{a_0^n}{n!}\,. \tag{8}$$

A couple of remarks are in order here: (i) we take for M [Eq. (8)] the smallest even integer such that the coefficient of a_0^M in $\mathcal{V}(a_0)$ is positive for all values of x_0 and β; this suffices to make the integral in (7) finite even when λ_0 vanishes; (ii) the factor $\lambda_0^{1/2}$ in $\mathcal{F}$ cancels the factor $\lambda_0^{-1/2}$ contained in $\Delta^{-1/2}$; combined with (i), this shows that the improved approximation to $\langle x_0|e^{-\beta\hat{H}}|x_0\rangle$, Eq. (6), is finite at the caustics; (iii) there is a one-to-one correspondence between the minima of $S[x]$ and the minima of $\mathcal{V}(a_0)$; therefore, it is not necessary to explicitly add their contributions as in (4), for they are already contained in $\mathcal{F}$.

Although the procedure outlined above teaches us how to cross the caustics, it is not very convenient: in order to obtain the coefficients of $\mathcal{V}(a_0)$ one has to find λ_0 and $\varphi_0(\tau)$. This, in general, is not an easy task, and makes the whole procedure very cumbersome. Instead, we shall present an alternative way of obtaining those coefficients, which is based on remark (iii) above.

Let us assume that $M = 4$ in Eq. (8); this is the case for the quartic double-well potential, to be discussed in the next section. Then the "effective action" $\mathcal{A}(a_0) \equiv S[x_{\rm gm}]+\mathcal{V}(a_0)$ for the "critical" mode φ_0 is a fourth degree polynomial in a_0. Let us assume it has three (real) extrema: a global minimum at $a_0 = 0$, a local maximum at $u > 0$, and a local minimum at $v > u$. This allows us to write such a polynomial as[5] $\mathcal{A}(a_0) = S[x_{\rm gm}] + \alpha\left[\frac{1}{2}\,uv\,a_0^2 - \frac{1}{3}\,(u+v)\,a_0^3 + \frac{1}{4}\,a_0^4\right]$. In order to relate the parameters in $\mathcal{A}(a_0)$ to calculable quantities, we impose that $\mathcal{A}(v) = S[x_{\rm lm}]$ and $\mathcal{A}(u) = S[x_{\rm sp}]$, where $x_{\rm lm}(\tau)$ and $x_{\rm sp}(\tau)$ are the local minimum and the lowest saddle-point of $S[x]$, respectively. This yields

$$\frac{S[x_{\rm lm}] - S[x_{\rm gm}]}{S[x_{\rm sp}] - S[x_{\rm gm}]} = \frac{\mathcal{A}(v) - \mathcal{A}(0)}{\mathcal{A}(u) - \mathcal{A}(0)} = \frac{\xi^3(2-\xi)}{2\xi - 1}, \tag{9}$$

where $\xi \equiv v/u$. Another combination of parameters which becomes determined is $\mu \equiv \alpha u^4$:

$$S[x_{\rm sp}] - S[x_{\rm gm}] = \mathcal{A}(u) - \mathcal{A}(0) = \frac{\mu}{12}\,(2\xi - 1). \tag{10}$$

[4]The procedure adopted here resembles the treatment of caustics in optics [5] and in quantum mechanics [6], suitably modified to take into account the Euclidean nature of the path integral in (2).

[5]One can easily check that $\mathcal{A}'(0) = \mathcal{A}'(u) = \mathcal{A}'(v) = 0$.

In terms of the calculable parameters ξ and μ, we can rewrite $\mathcal{A}(a_0)$ as $\mathcal{A}(a_0) = S[x_{\rm gm}] + \mathcal{V}_3(a_0/u)$, where $\mathcal{V}_3(z) = \mu\left[\frac{1}{2}\xi z^2 - \frac{1}{3}(1+\xi)z^3 + \frac{1}{4}z^4\right]$. There still remains one parameter to be determined, namely u. Fortunately, $\mathcal{F}$ does not depend on it. Indeed, identifying $\mathcal{V}_3(a_0/u)$ with $\mathcal{V}(a_0)$ yields $\lambda_0 = \mu\xi/u^2$, which allows us to rewrite (7) solely in terms of ξ and μ:

$$\mathcal{F} = \sqrt{\frac{\mu\xi}{2\pi\hbar u^2}} \int_{-\infty}^{\infty} da_0\, e^{-\mathcal{V}_3(a_0/u)/\hbar} = \sqrt{\frac{\mu\xi}{2\pi\hbar}} \int_{-\infty}^{\infty} dz\, e^{-\mathcal{V}_3(z)/\hbar}. \tag{11}$$

The discussion above can be easily adapted to the case in which $\mathcal{A}(a_0)$ has only one extremum. In this case, $\mathcal{A}'(a_0)$ has one real ($a_0 = 0$) and two complex conjugate roots (w and w^*), the latter corresponding to the *complex* trajectories $x_{\rm ct}(\tau)$ and $x^*_{\rm ct}(\tau)$. Accordingly, one has $\mathcal{A}(a_0) = S[x_{\rm gm}] + \mathcal{V}_1(a_0/|w|)$, where $\mathcal{V}_1(z) = \chi\left[\frac{1}{2}z^2 - \frac{2}{3}(\cos\phi)z^3 + \frac{1}{4}z^4\right]$, with $\chi \equiv \alpha|w|^4$ and $\phi \equiv \arg(w)$. Identifying $\mathcal{A}(w)$ with $S[x_{\rm ct}]$ then yields

$$S[x_{\rm ct}] - S[x_{\rm gm}] = \mathcal{A}(w) - \mathcal{A}(0) = \frac{\alpha w^3}{12}(2w^* - w) = \frac{\chi}{12}\left(2e^{2i\phi} - e^{4i\phi}\right), \tag{12}$$

from which we can obtain χ and ϕ. Finally, identifying $\mathcal{V}_1(a_0/|w|)$ with $\mathcal{V}(a_0)$ leads to $\lambda_0 = \chi/|w|^2$, so that

$$\mathcal{F} = \sqrt{\frac{\chi}{2\pi\hbar|w|^2}} \int_{-\infty}^{\infty} da_0\, e^{-\mathcal{V}_1(a_0/|w|)/\hbar} = \sqrt{\frac{\chi}{2\pi\hbar}} \int_{-\infty}^{\infty} dz\, e^{-\mathcal{V}_1(z)/\hbar}. \tag{13}$$

3 Application: the quartic double-well potential

Let us consider the quartic double-well potential, $V(x) = \frac{\lambda}{4}(x^2 - a^2)^2$, $\lambda > 0$. In order to simplify notation, we replace x and τ by $q \equiv x/a$ and $\theta \equiv \omega\tau$, respectively, where $\omega \equiv (\lambda a^2/m)^{1/2}$. In the new variables, the equation of motion reads $\ddot{q} = U'(q)$, where $U(q) = \frac{1}{4}(q^2-1)^2$. Closed trajectories have the form

$$q_{\rm c}(\theta) = q_{\rm t}\,\mathrm{cd}(u, k), \tag{14}$$

where cd is one of the Jacobian elliptic functions [7], $u \equiv \sqrt{1 - q_{\rm t}^2/2}\,(\theta - \Theta/2)$, $\Theta \equiv \beta\hbar\omega$, and $k \equiv \sqrt{q_{\rm t}^2/(2 - q_{\rm t}^2)}$. The turning point $q_{\rm t}$ is fixed by the boundary condition $q_{\rm c}(0) = q_0$. The classical action can be written as $S[x_{\rm c}] = (\hbar/g)\, I[q_{\rm c}]$, where $g \equiv \hbar\lambda/m^2\omega^3$ and

$$I[q_{\rm c}] = \Theta\, U(q_{\rm t}) + 2\,\mathrm{sgn}(q_{\rm t} - q_0) \int_{q_0}^{q_{\rm t}} \sqrt{2\left[U(q) - U(q_{\rm t})\right]}\, dq. \tag{15}$$

Finally, the determinant of the fluctuation operator is given by [2]

$$\Delta = 4\pi g\,\mathrm{sgn}(q_0 - q_{\rm t})\, \frac{\sqrt{2\left[U(q_0) - U(q_{\rm t})\right]}}{U'(q_{\rm t})} \left(\frac{\partial q_0}{\partial q_{\rm t}}\right)_\Theta. \tag{16}$$

Using these ingredients one can compute both the usual and the improved semiclassical approximations to $\langle q_0|e^{-\beta\hat{H}}|q_0\rangle$, Eqs. (4) and (6), respectively. The results are compared in Fig. 1.

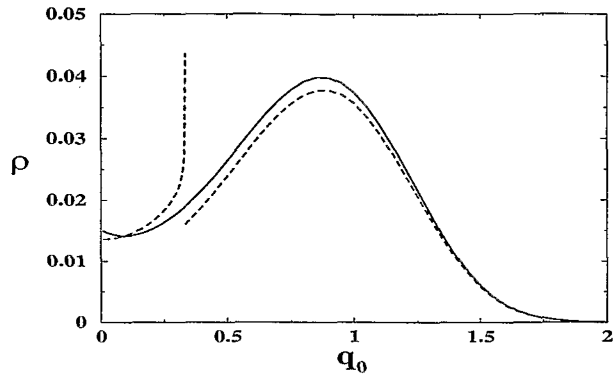

Figure 1: $\rho \equiv \langle q_0|e^{-\beta\hat{H}}|q_0\rangle$ *vs.* q_0 for $\Theta = 5.0$ and $g = 0.3$. The dashed line is obtained using the usual semiclassical approximation [Eq. (4)]; the solid line is the result of the approximation discussed in Section 2. The equation $q_c(0) = q_0$ (which determines the turning point q_t) has three real solutions for $q_0 < \tilde{q}_0 = 0.33319\ldots$; as we cross the caustic, two of them (the ones associated with a local minimum and a saddle-point of the action) coalesce — thus causing the divergence in the usual semiclassical approximation — and reemerge at the other side as a pair of complex conjugate solutions.

References

[1] R. P. Feynman, *Statistical Mechanics* (Addison-Wesley, New York, 1972); H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics* (World Scientific, Singapore, 1995).

[2] C. A. A. de Carvalho, R. M. Cavalcanti, E. S. Fraga, and S. E. Jorás, Ann. Phys. (N.Y.) **273**, 146 (1999); Phys. Rev. E **61**, 6392 (2000).

[3] C. A. A. de Carvalho and R. M. Cavalcanti, Braz. J. Phys. **27**, 373 (1997).

[4] J. Ankerhold and H. Grabert, Physica A **188**, 568 (1992); F. J. Weiper, J. Ankerhold, and H. Grabert, Physica A **223**, 193 (1996).

[5] M. Berry, in *Physics of Defects*, Les Houches Session XXXV (1980), edited by R. Balian, M. Kléman, and J.-P. Poirier (North-Holland, Amsterdam, 1981); M. V. Berry and C. Upstill, in *Progress in Optics XVIII*, edited by E. Wolf (North-Holland, Amsterdam, 1980).

[6] G. Dangelmayr and W. Veit, Ann. Phys. (N.Y.) **118**, 108 (1979); L. S. Schulman, *Techniques and Applications of Path Integration* (John Wiley, New York, 1981).

[7] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, New York, 1965).