Uniform approximation of wave functions with improved semiclassical transformation amplitudes and Gram-Schmidt orthogonalization

Edward D. Davis*
Department of Physics, Kuwait University, P.O. Box 5969, Safat, Kuwait
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Semiclassical transformation theory implies an integral representation for stationary-state wave functions $\psi_m(q)$ in terms of angle-action variables (θ, J). It is a particular solution of Schrödinger's time-independent equation when terms of order $\hbar^2$ and higher are omitted, but the preexponential factor $A(q,\theta)$ in the integrand of this integral representation does not possess the correct dependence on q. The origin of the problem is identified: the standard unitarity condition invoked in semiclassical transformation theory does not fix adequately in $A(q,\theta)$ a factor which is a function of the action J written in terms of q and θ. A prescription for an improved choice of this factor, based on successfully reproducing the leading behavior of wave functions in the vicinity of potential minima, is outlined. Exact evaluation of the modified integral representation via the residue theorem is possible. It yields wave functions which are not, in general, orthogonal. However, closed-form results obtained after Gram-Schmidt orthogonalization bear a striking resemblance to the exact analytical expressions for the stationary-state wave functions of the various potential models considered (namely, a Pöschl-Teller oscillator and the Morse oscillator).

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Semiclassical transformation theory approximates various quantum probability amplitudes in terms of the generating functions of classical canonical transformations [1]. The theory is aesthetically very satisfying in the manner in which it exploits parallels between quantum mechanics and classical mechanics. It has also proved eminently useful. The basic relations for amplitudes in terms of generating functions, although more than 30 years old, are still central to current research [2,3].

A formal application of semiclassical transformation theory [1] implies that the bound states of a conservative system of one degree of freedom have actions $J_m (m=0,1,2,\ldots)$ given by the appropriate Bohr-Sommerfeld quantization condition and approximate configuration space wave functions

$$\psi_m(q) = N_m \int A(q,\theta)\exp[(i/\hbar)F_{cl}(q,\theta)]\phi_m(\theta)d\theta, \qquad (1)$$

where $F_{cl}(q,\theta)$ is the generating function of the first kind (see Chap. 9 in Ref. [4]) for the canonical transformation from conjugate Cartesian variables (q,p) to the angle-action variables (θ,J) for the system, the preexponential factor

$$\mathcal{A}(q,\theta) = \mathcal{A}_U(q,\theta) \equiv \left[\frac{-1}{2\pi i\hbar}\frac{\partial^2 F_{cl}}{\partial q\,\partial\theta}\right]^{1/2}, \qquad (2)$$

$\phi_m(\theta) \equiv (2\pi i\hbar)^{-1/2}\exp(iJ_m\theta/\hbar)$, and N_m is a normalization constant [5]. Equations (1) and (2) reduce to an acceptable result (namely, the WKB approximation) if the integral is evaluated in the $\hbar\to 0$ stationary phase approximation. However, if one attempts to go beyond the stationary phase approximation as contemporary studies do, then there are problems. As specialization of Eqs. (1) and (2) to various examples reveals (see below and Appendix C.2 in Ref. [6]), the q dependence of $\mathcal{A}_U$ is typically spurious. In particular, wave functions do not have well-defined parity under circumstances when this symmetry is expected.

The integral representation of Eq. (1) with the preexponential factor in Eq. (2) is a *particular* solution of Schrödinger's time-independent equation when terms of order equal to or greater than $\hbar^2$ are discarded, but the *general* solution (to this order) only constrains the preexponential factor $A(q,\theta)$ to be of the form [7]

$$\mathcal{A}_G(q,\theta) \equiv f(J(q,\theta))\mathcal{A}_U(q,\theta), \qquad (3)$$

where f is an arbitary differentiable function of $J(q,\theta) = -\partial F_{cl}/\theta$ [8]. I claim that, in the case of potentials displaying a single minimum, the factor $f(J(q,\theta))$ can be chosen so that the corresponding approximate wave functions have the desired q behavior in the vicinity of the potential's minimum. In the case of even potentials $V(q)$ (with a single minimum), this is enough to guarantee that wave functions have the right parity. No matter what choice of f is made, the preexponential factors $\mathcal{A}_U(q,\theta)$ and $\mathcal{A}_G(q,\theta)$ are indistinguishable if the $\hbar\to 0$ stationary phase approximation is invoked [because $J(q,\theta)$ is then replaced by the constant J_m].

The choice of preexponential factor $\mathcal{A}_U(q,\theta)$ guarantees that, in the limit $\hbar\to 0$, the corresponding kernel $\mathcal{K}_U(q,\theta) \equiv \mathcal{A}_U(q,\theta)\exp[(i/\hbar)F_{cl}(q,\theta)]$ in Eq. (1) is an element of a unitary transformation matrix (or a quantum probability amplitude). Although this is an appealing property, it is by no means obvious that it is appropriate as there is no rigorous unitary quantum-mechanical counterpart to transformations from Cartesian phase space variables to (conventional) angle-action variables. In fact, one implication of the previous paragraph is that it is permissible to insist that $\mathcal{K}(q,\theta) \equiv A(q,\theta)\exp[(i/\hbar)F_{cl}(q,\theta)]$ is an element of a unitary trans-

*Electronic address: davis@kuc01.kuniv.edu.kw

formation matrix in the limit $\hbar \to 0$. The upshot of the considerations below is that this unitarity condition must be supplemented by more information to fix the preexponential factor completely.

Support for the assertion above about the role of the factor $f(J(q,\theta))$ comes from consideration of some analytically soluble models: the simple harmonic oscillator (discussed in Ref. [7]), a Pöschl-Teller oscillator described by the potential $V(q)=V_0 \tan^2(\pi q/a)$ $(V_0>0)$ and the Morse oscillator with potential $V(q)=D[1-\exp(-q/d)]^2$ $(D,d>0)$. The Pöschl-Teller and Morse models, which are taken up in the present work, also force one to consider issues related to the contour of integration in Eq. (1).

For the example of the harmonic oscillator, eigenfunctions can be obtained by integrating over the full range of θ (modulo 2π) for which $F_{cl}(q,\theta)$ exists for the value of q under consideration [9]. Despite the apparent reasonableness of this prescription, it is inappropriate in the case of the Pöschl-Teller potential. The corresponding limits of integration would contain a q dependence [10] incompatible with the requirement that the resulting integral representation for eigenfunctions satisfies Schrödinger's time-independent equation when terms of order $\hbar^2$ and higher are dropped. (The q-dependent limits would give rise to error terms of order $\hbar$.)

What alternatives are there? The general formal considerations of Ref. [7] suggest that the kernel $\mathcal{K}(q,\theta)=A(q,\theta)\exp[(i/\hbar)F_{cl}(q,\theta)]$ in Eq. (1) can be thought of as a generating function for (approximate) wave functions in the sense that they are determined (up to multiplicative constants) by the coefficients of an expansion of $\mathcal{K}(q,\theta)$ in powers of $w\equiv e^{-i\theta}$. More precisely, if the Bohr-Sommerfeld quantization condition $J_m=(m+\mu/4)\hbar$ applies (m is a nonnegative integer and μ is the Maslov index), then, according to Eq. (10) in Ref. [7], the expansion reads

$$\mathcal{K}(q,\theta(w)) = w^{\mu/4}\sum_{m=0}^{\infty}\frac{\psi_m(q)}{\tilde{n}_m}w^m, \tag{4}$$

where $\theta(w)=i\ln w$ [with $|w|$ chosen so that the series in Eq. (4) converges] and the $\tilde{n}_m$'s are constants [introduced in the denominator to simplify Eqs. (5) and (6)]. The expansion in Eq. (4) implies that approximate wave functions can be written as the Schläfli-like contour integral

$$\psi_m(q) = \frac{\tilde{n}_m}{2\pi i}\oint\left(\frac{1}{w}\right)^{m+1+\mu/4} A(q,\theta(w)) \times\exp[(i/\hbar)F_{cl}(q,\theta(w))]dw, \tag{5}$$

where the (counterclockwise) contour of integration is a simple closed curve around a pole of order $m+1$ at $w=0$ which does not enclose any other singularities of the integrand.

Despite appearances, the integral representations in Eqs. (1) and (5) are closely related: since $J_m=(m+\mu/4)\hbar$ in $\phi_m(\theta)$, the integrand of Eq. (1) transforms into the integrand of Eq. (5) under the replacement of θ by $w=e^{-i\theta}$ as the variable of integration. Thus implicit in Eq. (5) is a choice of the contour of integration for the integral representation in Eq. (1). If possible, it should pass through the point(s) of stationary phase which yield the WKB approximation. I shall not attempt to be more explicit here, because, for the purposes of this paper, the Rodrigues formula implied by Eq. (4) [or the residue theorem applied to Eq. (5)], namely

$$\psi_m(q) = \frac{\tilde{n}_m}{m!}\frac{\partial^m}{\partial w^m}[w^{-\mu/4}\mathcal{K}(q,\theta(w))]_{w=0}, \tag{6}$$

is more useful than either of the above integral representations.

When one can distinguish between states of different parity (as in the Pöschl-Teller model), it is necessary to introduce separate kernels $\mathcal{K}_\varrho$ for the positive $(\varrho=0)$ and negative parity $(\varrho=1)$ states [obtained by making different choices of the factor $f(J(q,\theta))$]. An expansion in powers of $z\equiv e^{-i2\theta}$ is now appropriate, the expansion being

$$\mathcal{K}_\varrho(q,\theta(z)) = z^{(\mu/4+\varrho)/2}\sum_{m=0}^{\infty}\frac{\psi_{2m+\varrho}(q)}{\tilde{n}_{2m+\varrho}}z^m. \tag{7}$$

The associated Rodrigues formula expresses $\psi_{2m+\varrho}(q)$ in terms of the mth [*not* the $(2m+\varrho)$th] partial derivative of $z^{-(\mu/4+\varrho)/2}\mathcal{K}_\varrho(q,\theta(z))$ with respect to z (evaluated at $z=0$). A division into two classes of states can also be helpful for models which do not respect parity (see the discussion of the Morse oscillator below).

The harmonic oscillator problem furnishes evidence that expansions like that in Eq. (4) or Eq. (7) do, in fact, exist. Consistent with Eq. 20 in Ref. [7], the kernels of definite parity are

$$\mathcal{K}_\varrho(q,\theta) = y^\varrho(\cos\theta)^{-(1/2+\varrho)}\exp\left(-\frac{i}{2}y^2\tan\theta\right), \tag{8}$$

where the dimensionless variable $y\equiv\sqrt{m\omega/\hbar}\,q$ (m is the mass of the oscillator and ω its angular frequency). The expression which results on the substitution of $e^{-i2\theta}$ by z can be recast into the form

$$\mathcal{K}_\varrho = 2^{1/2+\varrho}z^{1/4+\varrho/2}e^{-y^2/2}\exp\left(-\frac{1}{4}\frac{\partial^2}{\partial y^2}\right)y^\varrho e^{zy^2} \tag{9}$$

suitable for expansion in powers of z [11]. Using the Maclaurin series in z for $y^\varrho e^{y^2 z}$ and the fact that the Hermite polynomial $H_n(y)=2^n\exp[-1/4(\partial^2/\partial y^2)]y^n$ [see Eq. (1) in Ref. [12]], Eq. (9) implies that

$$\mathcal{K}_\varrho = 2^{(\varrho+1)/2}\left(\frac{\pi\hbar}{m\omega}\right)^{1/4}z^{1/4+\varrho/2}\sum_{m=0}^{\infty}\frac{[(2m+\varrho)!]^{1/2}}{2^m m!}\varphi_{2m+\varrho}(q)z^k, \tag{10}$$

where the $\varphi_n(q)$'s are the exact normalized energy eigenfunctions of the simple harmonic oscillator $[\varphi_n=[m\omega/(\pi\hbar)]^{1/4}(2^n n!)^{1/2}H_n(y)e^{-y^2/2}]$. Since the Maslov index $\mu=2$ for the harmonic oscillator, Eq. (10) constitutes an explicit realization of Eq. (7).

The Pöschl-Teller oscillator is instructive, because unlike the example of the harmonic oscillator, the results obtained are not exact and so it is possible to assess the quality of the

approximation based on Eqs. (1) and (3). Although the relevant transformation from Cartesian phase variables to angle-action variables appears in textbooks (see, for example, Chap. 7 in Ref. [13]), the corresponding generating function of the first kind is not so readily available. The calculation of this generating function as the Legendre transform of Hamilton's characteristic function $W(q,J)$ for the Pöschl-Teller problem is straightforward but lengthy, it being necessary to treat separately each branch of the multiple-valued $W(q,J)$ for both signs of q. Fortunately, the result can be compactly expressed [in a form suitable for use in the Rodrigues formula implied by Eq. (7)] as follows:

$$F_{cl}(q,\theta) = iJ_s \ln\{[\sqrt{(1-e^{-i2\theta})^2 + 4\cos^2(\pi q/a)e^{-i2\theta}} + (1 - e^{-2i\theta})]/[2\cos(\pi q/a)]\}, \tag{11}$$

where the parameter $J_s \equiv a\sqrt{2mV_0}/\pi$ sets the scale for classical actions (m is again the mass of the oscillator). In Eq. (11), which holds for both signs of q and the pertinent ranges of θ (see Ref. [10]), it is understood that the positive branch of the square root and the principal value of the logarithm function are to be adopted [14]. Partial differentiation of $F_{cl}(q,\theta)$ with respect to θ [15] yields

$$J(q,\theta) \equiv -\frac{\partial F_{cl}}{\partial \theta} = J_s(\{1-[\sin(\pi q/a)\cos\theta]^2\}^{-1/2} - 1), \tag{12}$$

implying that, for the present problem, the factor $f(J(q,\theta))$ in $\mathcal{A}_G$ is, in effect, a function of the combination $\sin(\pi q/a)/\cos\theta$. Likewise, the second partial derivative of F_{cl} required in $\mathcal{A}_G$ (and $\mathcal{A}_U$),

$$\frac{\partial^2 F_{cl}}{\partial q\,\partial\theta} = -\frac{\pi}{a}J_s\cos(\pi q/a)\frac{\sin(\pi q/a)}{\cos^2\theta}\{1 - [\sin(\pi q/a)/\cos\theta]^2\}^{-3/2}, \tag{13}$$

amounts to the product of $\cot(\pi q/a)$ with a function of $\sin(\pi q/a)/\cos\theta$. preexponential factors must therefore be of the form $[\cot(\pi q/a)]^{1/2}G[\sin(\pi q/a)/\cos\theta]$, where G is some differentiable function. This functional form is compatible with choices which possess the leading small q behavior expected of energy eigenfunctions of definite parity, the *simplest* being

$$A_\varrho(q,\theta) = [\cot(\pi q/a)]^{1/2}\left[\frac{\sin(\pi q/a)}{\cos\theta}\right]^{1/2+\varrho} = [\cos(\pi q/a)]^{1/2}\frac{\sin^\varrho(\pi q/a)}{(\cos\theta)^{1/2+\varrho}}, \tag{14}$$

where, as above, $\varrho=0$ (1) for positive (negative) parity states. Equation (13) serves to illustrate that the preexponential factor $\mathcal{A}_U$ would have the wrong leading behavior for small q.

With the preexponential factors of Eq. (14), the Rodrigues' formula for approximate energy eigenfunctions implies that

$$\psi_{2m+\varrho}(q) \propto \left[\cos\left(\frac{\pi}{a}q\right)\right]^{\Lambda+1/2} P_m^{(\varrho)}[\sin(\pi q/a)], \tag{15}$$

where $\Lambda \equiv J_s/\hbar$ and

$$P_k^{(\varrho)}(x) \equiv x^\varrho \frac{d^k}{dz^k}[(1+z)^{-(1/2+\varrho)}(1-z+\sqrt{(1+z)^2-4x^2z})^{-\Lambda}]_{z=0} \tag{16}$$

is a polynomial of order $2k+\varrho$ and well-defined parity $[P_k^{(\varrho)}(-x)=(-1)^\varrho P_k^{(\varrho)}(x)]$. Calculation shows that these approximate wave functions are *not* orthogonal although the degree of nonorthogonality is slight if $\Lambda \gg 1$ [16]. In terms of $x=\sin(\pi q/a)$, orthogonalization amounts to the construction of a set of orthogonal polynomials on the interval $-1<x<+1$ with weight function $(1-x^2)^\Lambda$. This is the set of ultraspherical polynomials $C_n^{(\Lambda+1/2)}(x)$ [17]. Accordingly, after orthonormalization, the approximate wave functions are

$$N_n(\Lambda)[\cos(\pi q/a)]^{\Lambda+1/2}C_n^{(\Lambda+1/2)}[\sin(\pi q/a)], \tag{17}$$

where the $N_n(\Lambda)$'s are normalization constants ($n=0,1,2,\ldots$). Remarkably, the exact energy eigenfunctions [18] are also given by Eq. (17) with Λ replaced by $\sqrt{\Lambda^2+1/4}$.

The analytic expressions for the nonorthogonal wave functions in Eq. (15) and the orthogonalized wave functions in Eq. (17) do not appear to be significantly different: barring the overall normalization factors, the coefficients of each power of $x=\sin(\pi q/a)$ agree to leading order in Λ (see Ref. [19] for some examples). Nevertheless, orthogonalization is crucial. Numerical studies reveal that it improves substantially the agreement between approximate and exact eigenfunctions (so that it is good provided $\Lambda^2 \gg 1$). Perhaps more telling is the fact that, even when $\Lambda \gg 1$, the nonorthogonal wave functions can be inferior to (approximately) normalized WKB wave functions [20] inside the classically allowed region (well away from the classical turning points).

Analysis of the Morse oscillator serves to illustrate that it is possible to treat models which do not possess wave functions of good parity. The guiding principle I have found useful is to insist that, in the immediate vicinity of the potential minimum (at $q=0$), the approximate Morse oscillator wave functions $\tilde{\psi}_n(q)$ resemble those of a harmonic oscillator of the same mass m and the appropriate angular frequency, namely $\tilde{\omega}=\tilde{J}_s/(md^2)$ where the action $\tilde{J}_s \equiv \sqrt{2mD}d$ [21]. Not only is the preexponential factor $A(q,\theta)$ at issue but also the analytic continuation to complex values of θ of the generating function $F_{cl}(q,\theta)$ to be used in Eqs. (5) or (6) and even the choice of $F_{cl}(q,\theta)$ for real values of θ [22]. Adoption of the $q>0$ result for $F_{cl}(q,\theta)$ is indicated, which, for $0<\theta<\pi$, reads

$$F_{cl}(q,\theta) = \tilde{J}_s\{\sqrt{\lambda^2(q,\theta)-(1-e^{-q/d})^2} + \arccos[(1 - e^{-q/d})/\lambda(q,\theta)] - \theta\}, \tag{18}$$

where $\lambda(q,\theta)$ is the positive root of the relation $q/d=\ln[(1+\lambda\cos\theta)/(1-\lambda^2)]$ and arccos denotes the principal value of the inverse cosine function. It is understood that the principal values of all square roots present either explicitly or implic-

itly [in $\lambda(\theta,q)$] are to be used. The analytic continuation (of interest) of $F_{cl}(q,\theta)$ to complex θ is such that the alternative branch of the square root $\sqrt{\lambda^2(q,\theta)-(1-e^{-q/d})^2}$ in Eq. (18) is adopted [23].

In view of the fact that I compare Morse oscillator wave functions with those of the harmonic oscillator, it is still useful to divide them into a $\varrho=0$ class $\{\widetilde{\psi}_{2m}(q)\}$ and a $\varrho=1$ class $\{\widetilde{\psi}_{2m+1}(q)\}$, which correspond (near $q=0$) to the positive and negative parity harmonic oscillator wave functions, respectively ($m=0,1,\ldots$). Suitable preexponential factors for the two classes of wave functions are $[e^{-2q}\cos^2\theta+4(1-e^{-q})]^{-1/4}\widetilde{G}_{\varrho}(\lambda(q,\theta))$, where the simplest appropriate choice of $\widetilde{G}_{\varrho}(x)$ is $\widetilde{G}_{\varrho}(x)=x^{\varrho}$. For this choice, the approximate energy eigenfunctions are found to be of the form

$$\widetilde{\psi}_n(q) \propto (e^{-q/d})^{\widetilde{\Lambda}-n-1/2}\exp(-\widetilde{\Lambda}e^{-q/d})\widetilde{P}_n(e^{-q/d}), \qquad (19)$$

where $\widetilde{P}_n(x)$ is a polynomial of order n and $\widetilde{\Lambda}\equiv\widetilde{J}_s/\hbar$. As in the case of the Pöschl-Teller oscillator, the wave functions $\widetilde{\psi}_n(q)$ in Eq. (19) are slightly nonorthogonal. After orthonormalization, the exact bound-state wave functions [24] are obtained.

In summary, the examples in this paper illustrate just how much can be learned about wave functions of simple systems using a modification of the approximate integral representation in Eq. (1). One change seeks to correct for obvious deficiencies of the preexponential factor implied by semiclassical transformation theory [namely, $\mathcal{A}_U$ in Eq. (2)]. Other changes may appear less welcome but are equally essential: the use of a complex-valued contour of integration and, sometimes, an appropriate analytic continuation of the generating function. Despite the lack of intuitive appeal inherent in the use of a complex-valued contour, it does facilitate analytic evaluation of the integral representation (since the residue theorem may be invoked). Typically, semiclassical integral representations improving on Eq. (1) entail integration over classical trajectories [25–27]. This is one obvious difference between these representations and the one explored here. There is another. Corrections to the preexponential factor have been guided in this work by the structure of the general solution in Eq. (3). This approach is inappropriate for integral representations involving integration over classical trajectories: the factor $f(J(q,\theta))$ in Eq. (3) becomes an invisible constant [since $J(q,\theta)$ is equal to the fixed action on a trajectory].

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[1] W. H. Miller, Adv. Chem. Phys. **25**, 69 (1974).
[2] W. H. Miller, J. Phys. Chem. A **105**, 2942 (2001).
[3] K. G. Kay, J. Phys. Chem. A **105**, 2535 (2001).
[4] H. Goldstein, *Classical Mechanics*, 2nd ed. (Addison-Wesley, Reading, MA, 1980).
[5] I have adopted the phase conventions of Ref. [1] in defining $A(q,\theta)$ and $\phi_m(\theta)$.
[6] M. S. Child, *Semiclassical Mechanics with Molecular Applications* (Clarendon Press, Oxford, 1991).
[7] E. D. Davis and G. I. Ghandour, Phys. Lett. A **309**, 1 (2003).
[8] The eigenenergies are $E_m\equiv K(J_m)$, where $K(J)$ is the classical Hamiltonian function for angle-action variables.
[9] This is illustrated by Eqs. (C.62a,b) in Appendix C of Ref. [6] , where the integration is from $\theta=-\pi/2$ to $\theta=+\pi/2$. This interval corresponds to the full range of values of θ (modulo 2π) for which $F_{cl}(q,\theta)$ exists when $q>0$. For $q<0$, $F_{cl}(q,\theta)$ exists when $\pi/2<\theta \bmod 2\pi<3\pi/2$. However, the integrands of the integral representations in Eqs. (C.62a,b) of Ref. [6] are periodic with period π. (The definition of the variable θ in Ref. [6] and in the present paper is such that $\theta=0$ when $p=0$ and $q>0$.)
[10] In the case of the Pöschl-Teller potential, $F_{cl}(q,\theta)$ exists for $-\psi_q<\theta \bmod 2\pi<+\psi_q$ when $q>0$ and for $\pi-\psi_q<\theta \bmod 2\pi<\pi+\psi_q$ when $q<0$, where $\psi_q\equiv\pi/2-(\pi/a)|q|$. These restrictions on θ emerge in the construction of $F_{cl}(q,\theta)$ as the Legendre transform of Hamilton's characteristic function for this potential.
[11] Writing the Gaussian $e^{-\alpha y^2}$ in terms of its Fourier transform, one can prove that

$$\exp\left(-\frac{1}{4}\frac{\partial^2}{\partial y^2}\right)y^{\varrho}e^{-\alpha y^2}=\frac{y^{\varrho}}{(1-\alpha)^{\varrho+1/2}}\exp\left[\frac{\alpha y^2}{1-\alpha}\right]$$

for $\alpha>0$ and $\varrho=0,1$. The analytic continuation of this identity to arbitary $\alpha(=-z)$ is invoked in the steps leading to Eq. (9).
[12] F. M. Fernández, Phys. Lett. A **237**, 189 (1998).
[13] I. Percival and D. Richards, *Introduction to Dynamics* (Cambridge University Press, Cambridge, England, 1982).
[14] The expression in Eq. (11) is a little disconcerting inasmuch as it is not immediately apparent that $F_{cl}(q,\theta)$ is real valued. However, it is possible to infer manifestly real expressions if one considers q of a definite sign and restricted ranges of θ. For example, for $q>0$ and $|\theta|<\pi/2-\pi q/a$, Eq. (11) reduces to $F_{cl}=J_s\{\theta-\arcsin[\sin\theta/\cos(\pi q/a)]\}$, where arcsin denotes the principal value of the inverse sine function.
[15] Calculation of this partial derivative starting from Eq. (11) is awkward. Instead, one can take advantage of the fact that the expression in Eq. (11) is an even function of q (for fixed θ) and periodic in θ with period π (for fixed q) to use the form of $F_{cl}(q,\theta)$ given in Ref. [14] . Equation (12) for $J(q,\theta)$ can also be obtained without knowledge of $F_{cl}(q,\theta)$ by using the relation for q in terms of angle-action variables, namely $q=(a/\pi)\arcsin\{[1-1/(1+J/J_s)^2]^{1/2}\cos\theta\}$.
[16] If Θ is the angle between two wave functions defined using inner products, then $\cos\Theta$ is of the order of $1/\Lambda$.
[17] Ultraspherical or Gegenbauer polynomials are discussed in, for example, *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (U.S. GPO, Washington, DC, 1964), Chap. 22.

[18] G. Pöschl and E. Teller, Z. Phys. **83**, 143 (1933); F. Gori and L. de la Torre, Eur. J. Phys. **24**, 1 (2003).
[19] J. Al-Modhayan, M.S. dissertation, Kuwait University, 2002.
[20] Approximate normalization is achieved by employing the simple estimate given in Eq. (2.78) in M. Brack and R. K. Bhaduri, *Semiclassical Physics* (Addison-Wesley, Reading, MA, 1997).
[21] In making this demand, I am implicitly taking advantage of the fact that the semiclassical method under consideration is exact for the simple harmonic oscillator.
[22] The Morse oscillator generating function $F_{cl}(q,\theta)$ is single valued for $q>0$ but double valued for $q<0$. For $q>0$, $0 \leqslant \theta \bmod 2\pi < \pi$, while for $q<0$, $\psi_{cr} \leqslant \theta \bmod 2\pi < \pi$, where, in terms of $\lambda_{cr} \equiv \sqrt{e^{-q/d}-1}$, ψ_{cr} $(>\pi/2)$ is such that $\tan(\psi_{cr}/2)=(1+\lambda_{cr})/(1-\lambda_{cr})$. (As $q/d>-\ln 2$ for bound trajectories, reality of λ_{cr} is guaranteed).
[23] This choice of branch implies that the term $\widetilde{\Lambda}e^{-q/d}$ in the argument of the global exponential factor $\exp[-(\widetilde{\Lambda}-n-1/2)q/d - \widetilde{\Lambda}e^{-q/d}]$ in Eq. (19) is preceded by a minus sign. As a result, the quadratic small q approximation to this exponential factor, taking into account only those terms in the argument linear in $\widetilde{\Lambda}$ $(\gg 1)$, is proportional to the quadratic small q approximation to the Gaussian factor $\exp[-m\widetilde{\omega}q^2/(2\hbar)]=\exp[-\widetilde{\Lambda}q^2/(2d^2)]$ common to all wave functions of the related harmonic oscillator problem.
[24] P. M. Morse, Phys. Rev. **34**, 57 (1929); L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon, Oxford, 1965), pp. 72–3.
[25] R. G. Littlejohn, Phys. Rev. Lett. **56**, 2000 (1986).
[26] D. Zor and K. G. Kay, Phys. Rev. Lett. **76**, 1990 (1996).
[27] M. Madhusoodanan and K. G. Kay, J. Chem. Phys. **109**, 2644 (1998).