PHYSICAL REVIEW D VOLUME 25, NUMBER 6 15 MARCH 1982

Bohr-Sommerfeld quantization with the effective action variable

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(Received 13 August 1979; revised manuscript received 13 October 1981)

The effective action variable with its attendant modified potential is applied herein to the bound state, for which it is hypothesized that the Bohr-Sommerfeld whole-integer quantization is correct. Results for various one-dimensional potentials support this hypothesis. Finite turning points for bound-state effective action integrands do not exist. Also, it is shown that the modified potential for bound states is not unique.

I. INTRODUCTION

Old quantum theory was discarded because the Bohr-Sommerfeld quantization, Nh, of the classical action variable was inconsistent with observation. The semiclassical quantization of the WKB approximation, which includes the additional half-integer term $\frac{1}{2}h$ as a first correction, remains nonetheless limited by its asymptotic character. Recently, the phase-integral approximation has been modified by incorporating a first-principles modified potential whose expansion to various orders has been investigated.[1,2] In one dimension x, this modified potential U is determined from the potential V by the nonlinear differential equation[1,2]

$$U+\frac{\hbar^2}{8\mu}\frac{U''}{E-U}+\frac{5\hbar^2}{32\mu}\left[\frac{U'}{E-U}\right]^2=V(x)\ , \tag{1}$$

where E is the energy, $\hbar$ is Planck's constant, and μ is the mass. For $V(x)$ remaining finite for finite x, the boundary condition for Eq. (1) for bound states is that $U(x)<E$ for all finite x and that $U(x)\rightarrow E$ asymptotically from below as $x\rightarrow\pm\infty$. Equation (1) had been previously derived[1,2] by substituting for the wave function ψ an ansatz of the form

$$\psi(x)=[E-U(x)]^{-1/4}\exp\left[\pm i\int^x\left[\frac{2\mu}{\hbar^2}[E-U(x')]\right]^{1/2}dx'\right]$$

into the one-dimensional time-independent Schrödinger equation in order to generate an equation for our new unknown function $U(x)$. An effective action variable J is defined as follows:

$$J=\oint\{2\mu[E-U(x)]\}^{1/2}dx\ , \tag{2}$$

where the integral path is over one period (either libration or rotation). An effective momentum p is defined by the integrand of Eq. (2)—i.e., $p=[2\mu(E-U)]^{1/2}$.

The objectives of this exposition are three in number. The first objective is to extend the effective action variable to bound states (libration). An initial application of the effective action variable to cases of rotation has already been given where for Bloch quantization the effective action variable for periodic boundary conditions renders accurate results.[1,2] The second objective is to examine the hypothesis that the Bohr-Sommerfeld whole-integer quantization is correct, that is $J=Nh$ where E is specified to be the Nth energy eigenvalue (ground level E is specified by $N=1$) of the potential. And the third objective is to demonstrate that the modified potential is not necessarily unique.

From the boundary conditions for Eq. (1) for $V(x)$ remaining finite for finite x, the existence of finite turning points of the integrand of Eq. (2) (i.e., $p=0$) are precluded in principle for a complete solution of the modified potential. Even for simple one-dimensional potentials, closed-form solutions for the modified potential are regrettably not known. Asymptotic series expansions of the modified potential, which were successful when applied to a nearly free electron in a periodic potential,[2] are degraded in application to bound states, especially for ground states. Furthermore, any addition of the general solutions to the particular

solution for the expansion of the modified potential (to demonstrate the nonuniqueness of the modified potential) necessitates that the consequent effective action variable be evaluated numerically [this numerical procedure is not competitive with a Runge-Kutta solution of Eq. (1)]. Nevertheless, we report but do not show herein that the results for these series expansions with Bohr-Sommerfeld whole-integer quantization do compare with WKB results with half-integer quantization.

In Sec. II, we present our analyses. The supporting numerical analysis is reported in a supplement.[3] In Sec. III, we present a discussion that includes both a development of a modified Hamilton-Jacobi representation and a process to recover the Schrödinger wave equation.

II. ANALYSES

Since the wave function in one dimension is real (except for an unimportant phase factor),[4] we may choose a trigonometric representation for our ansatz such that

$$\Psi(x)=[E-U(x)]^{-1/4}\sin\left[\int_{-\infty}^{x}\left[\frac{2\mu}{\hbar^2}[E-U(x')]\right]^{1/2}dx'\right]$$

in order that $\Psi(x)\rightarrow 0$ for bound states as $x\rightarrow\pm\infty$. When this trigonometric ansatz is substituted into the time-independent Schrödinger equation, we still obtain Eq. (1). Our trigonometric ansatz will have $\Psi(x)\rightarrow 0$ at $x\rightarrow\infty$ if for energy eigenvalues E for the potential $V(x)$ we have that

$$\frac{J}{2\hbar}=\int_{-\infty}^{\infty}\left[\frac{2\mu}{\hbar^2}[E-U(x)]\right]^{1/2}dx=N\pi,\quad N=1,2,3,\ldots$$

which is the Bohr-Sommerfeld whole-integer quantization. We now demonstrate that this Bohr-Sommerfeld whole-integer quantization is consistent with our nonunique solutions to Eq. (1) for the modified potential $U(x)$.

In the absence of closed-form solutions for the modified potential and the degradation of asymptotic series expansions for bound-state modified potentials, we herein numerically substantiate the Bohr-Sommerfeld whole-integer quantization hypothesis by applying the Runge-Kutta method to a transformation of Eq. (1) in order to compute nonunique modified potentials. We first test the quantization hypothesis on the one-dimensional harmonic oscillator. This oscillator is a most stringent test for Bohr-Sommerfeld whole-integer quantization since the WKB half-integer quantization, which explicitly has its quantization in exact opposition, $\hbar/2$, with respect to the mantissa for modulo h vis-a-vis the Bohr-Sommerfeld quantization, fortuitously renders exact results. To show that the harmonic oscillator is not a unique case, we apply this numerical procedure to other one-dimensional potentials including a symmetric bilinear potential, a quartic potential, and a nonsymmetric Morse potential. This numerical analysis is developed in the supplement.[3] Convergence to whole-integer quantization of the effective action variable for various nonunique modified potentials extends down to the ground state. The relative error of this numerical process, which has been driven to the limits of our machine, is of the order of 10^{-9}. Furthermore, the rate of convergence, until limited by machine round-off, is consistent with the expected rate in accordance with Runge-Kutta step size and supports Richardson extrapolation.[5] For modified potentials that are numerically derived by the Runge-Kutta method, finite turning points for the effective action integrand for bound states do not exist. This condition removes any need for the traditional encumbrance associated with turning points such as connecting formulas, Stoke's phenomenon, and contour path selection. In all cases investigated, $U(x)$ numerically approaches E asymptotically from below both as $x\rightarrow+\infty$ in a manner which suggests[6] critical-point behavior of the stable-node class and as $x\rightarrow-\infty$ in a manner which suggests unstable-node behavior. This stable-node behavior of U may be substantiated for $x\rightarrow\infty$ by considering that for sufficiently large x in the classically forbidden region [i.e., $V(x)>E$], there exists an $x_0<x$ with x_0 also in the classically forbidden region such that we may approximate $U(x)$ by

$$U \approx E - K[V(x)-E]\exp\left[-\int_{x_0}^{x} 4\left[\frac{2\mu}{\hbar^2}[V(x')-E]\right]^{1/2} dx'\right],$$

where K is some arbitrary positive constant if (for sufficiency only) $(d/dx)\ln V(x) \sim O(1/x)$. This approximation improves as $x_0 \to \infty$. The analogy for $x \to -\infty$ is similar.

Three sample numerical modified potentials $U(x)$, which are developed in the supplement,[3] for the ground-state harmonic oscillator $V(x)=\mu\omega^2 x^2/2$ are exhibited in Fig. 1. We report port in the supplement[3] but do not exhibit on Fig. 1 that nonsymmetric modified potentials [i.e., $u'(0)\neq 0$] which also rendered the whole-integer quantization of Eq. (2) were also generated for the ground state of the harmonic oscillator. The behavior of the modified potential is exhibited for the lowest three energy eigenvalues of the harmonic oscillator in Fig. 2. Note the nodal behavior of V as $x \to \pm\infty$ in Figs. 1 and 2.

By numerical analysis in the supplement, it is also shown that the effective action variable has nearly the same functional dependence upon E as that for the classical action variable.

III. DISCUSSION

The convergence of the numerical results for the various cases and the consistent rate of convergence as a function of Runge-Kutta step size strongly support both the hypothesis that the whole-integer Bohr-Sommerfeld quantization is correct for the effective action variable and the fact that the modified potential is not unique.[3]

The modified potential method has been applied to wave propagation where a rigorous theory of geometric ray propagation, which is innately dependent upon wave number by an effective index of refraction, has been developed for continuous media from first principles.[7] Essentially this application has extended the Hamilton-Jacobi theory to the domain of propagation of waves of finite wavelength. For WKB quantization it is reasonable to attribute the missing half-wavelength to exponential penetration by the wave into the classical forbidden region beyond the turning point in this semiclassical theory. In the case of a known modified potential the correct orbital trajectory (or ray path with its associated known effective index of refraction) is also known. Thus the need for compensation for penetration beyond the turning points, which have receded from finite x space for known modified potentials if $V(x)$ remains finite for finite x, does not exist. Consequently the Bohr-Sommerfeld quantization stands.

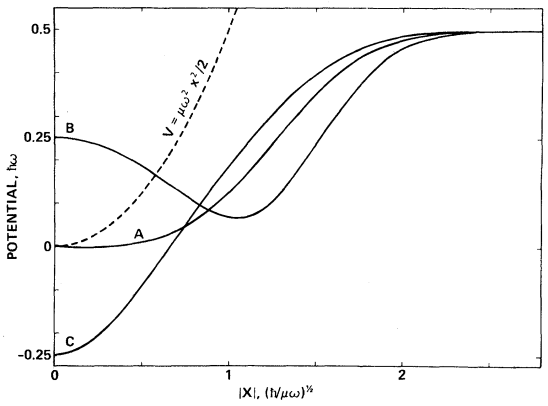

FIG. 1. Some of the various modified potentials for the ground state of the harmonic oscillator are represented by solid lines. Label A identifies the curve that is generated from the set of conditions that $U(0)=0$ and $U'(0)=0$; B, from $U(0)=0.25\hbar\omega$ and $U'(0)=0$; and C, from $U(0)=-0.25\hbar\omega$ and $U'(0)=0$. The actual potential for the harmonic oscillator is represented by the dashed curve.

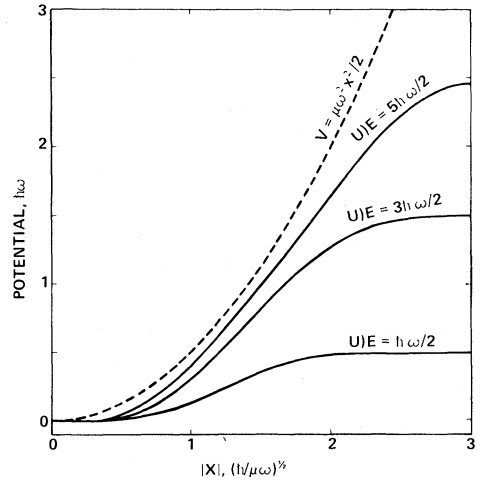

FIG. 2. Modified potentials for case A [generated from the set of conditions that $U(0)=0$ and $U'(0)=0$] for the ground state and first two excited states of the harmonic oscillator are represented by the solid lines. The actual potential for the harmonic oscillator is represented by the dashed curve.

Consistent with the correspondence principle, we see by Eq. (1) that if $\mu \to \infty$, $E \to \infty$, or $h \to 0$, then $U \to V$. Equation (1) makes the adjustment in one dimension so that the Hamilton-Jacobi theory may be extended into the quantum domain by using the modified potential as the continuation of potential. Here instead of stressing the wave properties of the particle and solving the wave equation, we adjust the potential for the wave character of the ideal but unrealizable infinitesimal test charge (i.e., a generalized charge consistent with the particular field) used for establishing the field associated with the potential. This procedure ensures that the test charge itself in the infinitesimal limit would not distort the field.[8] As this infinitesimal limit cannot be realized, workers have extrapolated the particular field from measurements with small but finite test charges. The modified potential corrects for the errors innate to this extrapolation.

Bohr-Sommerfeld quantization is limited to periodic or multiply periodic systems. The modified potential is not so limited. However, determination of the consequent stationary trajectories must include the effects of the Heisenberg uncertainty principle at the end points. Had we been somehow given the initial conditions for both the effective momentum and its derivative at a position anywhere along the trajectory (or orbit) in effective phase space (i.e., space formed by effective momentum coordinates and spatial coordinates), we would have determined the modified potential as an initial value problem so that Huygens's construction of wave fronts (albeit of one spatial dimension) could be achieved in the immediate neighborhood (for Huygens's construction of wave fronts in three dimensions with an effective index of refraction, see Ref. 7) and the effective momentum could be determined at all other points of the trajectory (or orbit). For example, case A of Fig. 1 represents the initial conditions $U(0)=0$ and $U'(0)=0$ for the ground state of the harmonic oscillator.

We can recover the Schrödinger wave function ψ through the ansatz. For the ground state of the harmonic oscillator, we could choose U to be case A [generated from the set of conditions that $U(0)=0$ and $U'(0)=0$] of Fig. 1. If U is only known approximately, then an approximation ϕ for ψ may be expressed for the ground state as follows:

$$\phi = C_1 (E-U)^{-1/4} \cos\left[\int_0^x \frac{1}{\hbar}[2\mu(E-U)]^{1/2} dy\right],$$

where C_1 is the ground-state normalization. The actual ground-state wave function ψ is then expressed as

$$\psi = (\mu\omega/\hbar)^{1/2} \pi^{-1/4} \exp\left[\frac{-\mu\omega x^2}{2\hbar}\right].$$

Let the normalization be $C_1 = \omega^{3/4}\hbar^{-1/4}$ for the ground state. Then $\phi(0)=\psi(0)$. For a Runge-Kutta step size of 0.001 $(\hbar/\mu\omega)^{1/2}$, the two fractional errors $[\psi(x)-\phi(x)]/\psi(0)$ and $[\psi(x)-\phi(x)]/\psi(x)$ are exhibited semilogarithmically as a function of $|x|$ on Fig. 3. The excellent accuracy through the WKB turning point and well out into the tail may be compared to the WKB results of Fröman and Mrazek,[9] which blow up at the WKB turning points.

Let us briefly discuss the cost for obtaining a bound-state energy eigenvalue. At first glance, the cost here appears to be prohibitive relative to traditional means where in order to determine the energy eigenvalue of V one must solve a second-order linear differential equation (i.e., the Schrödinger equation) subject to certain boundary conditions. Here we solve a second-order nonlinear differential equation [i.e., Eq. (1)] subject to similar boundary conditions and subsequently the solution to Eq. (1) must be applied to Eq. (2) in order to determine the energy eigenvalue. However, there are two cir-

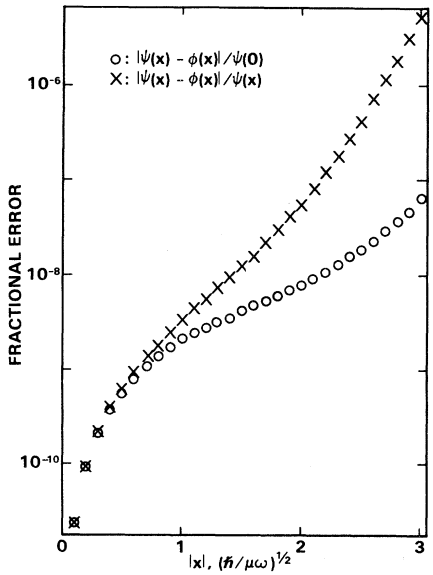

FIG. 3. The fractional error for the recovered wave function of the ground state of the harmonic oscillator is exhibited on semilogarithmic format for modified potentials derived with a Runge-Kutta step size of 0.001 $\times(\hbar/\mu\omega)^{1/2}$. The leading contribution to the fractional error is due to machine round-off.

cumstances that alleviate this apparent prohibitive cost. First, the nodal behavior of $U(x)$ as $x \to \pm\infty$ allows us to satisfy the boundary conditions of Eq. (1) trivially (the Schrödinger wave function does not enjoy a similar critical-point behavior that trivially satisfies its boundary conditions). And second, as the effective action variable nearly mimics the behavior of the classical action variable as a function of energy, we may easily converge to the energy eigenvalue by employing shooting techniques to Eq. (2). In actual practice when numerical techniques are needed for one-dimensional wave mechanics, our technique as described herein becomes competitive.

For the record, the quantization advanced herein differs from Dunham's whole-integer quantization[10]

$$\frac{1}{i2\pi}\oint \sum_{j=0}^{\infty} h^j S_j' dx = mh \quad (m=0,1,2,\ldots),$$

where S_j' is an element of the WKB asymptotic series: $S_0' = [2\mu(E-V)]^{1/2}$, etc. Note that Dunham's quantization is related to the finite WKB turning points. The evaluation of $\oint hS_1' dx$ gives the half-integer quantization, which manifests the usual WKB amplitude factor, and higher odd-j terms vanish[11] when integrated around the closed contour. Thus Dunham's asymptotic quantization becomes the usual[11]

$$\frac{1}{i2\pi}\oint \sum_{j=0}^{\infty} h^{2j} S_{2j}' dx = (m+\tfrac{1}{2})h \quad (m=0,1,2\ldots).$$

Had we so chosen to manifest the amplitude factor of our ansatz for ψ of Ref. 2 as a logarithmic term in the exponent in order to develop our analogy to Dunham, then Eq. (1) would remain valid and our analogous quantization would become a half-integer quantization expressed as follows:

$$\oint \left[[2\mu(E-U)]^{1/2} + \frac{i}{2}\frac{d}{dx}\ln[2\mu(E-U)]^{1/2} \right] dx = (N-\tfrac{1}{2})h \quad (N=1,2,3,\ldots),$$

where the branch points are $x = \pm\infty$ and where the logarithmic term would contribute the half-integer term.

ACKNOWLEDGMENT

This work was supported in part by the Independent Research Program of the Naval Ocean Systems Center.

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