Semiclassical wave equation and exactness of the WKB method

M. N. Sergeenko

The National Academy of Sciences of Belarus, Institute of Physics, Minsk 220072, Belarus

Abstract

The exactness of the semiclassical method for three-dimensional problems in quantum mechanics is analyzed. The wave equation appropriate in the quasiclassical region is derived. It is shown that application of the standard leading-order WKB quantization condition to this equation reproduces exact energy eigenvalues for all solvable spherically symmetric potentials.

PACS number(s): 03.05.Ge, 03.65.Sq

1. Introduction

There are several problems in quantum mechanics that can be solved exactly in terms of special functions. However, the same problems can be solved exactly also in terms of elementary functions in the framework of the WKB method.

The WKB method was originally proposed for obtaining approximate eigenvalues of one-dimensional Schrödinger problems in the limiting case of large quantum numbers. At present, the WKB method is important and intriguing by its simplicity and efficiency, a powerful tool of investigation not only in quantum mechanics but also in many other branches of theoretical physics, for example, in the theory of electromagnetic waves. In several common applications the method gives very accurate results. However, from the moment of its appearance up to now the same old problem of exactness of the WKB approximation has arisen.

The structure of supersymmetric quantum mechanics motivates a modified semiclassical quantization condition for one-dimensional Hamiltonians [1, 2]. The supersymmetric WKB (SWKB) method is a modification of the standard WKB quantization for obtaining the quasiclassical eigenvalues of nonrelativistic Hamiltonians. It was demonstrated [4]-[5] that the modified leading-order SWKB quantization condition in each and every case reproduces the exact energy eigenvalues for a class of solvable potentials. For these models the solutions can be written in terms of elementary functions.

Recent successes of the SWKB quantization rule have revived interest in the original WKB quantization condition. Proofs of varying degrees of rigor have been advanced that demonstrate the exactness of the standard WKB quantization condition [6]-[12]. In Ref. [12], a modification of the standard WKB approximation has been considered for which the leading-order quantization condition determines the exact energy eigenvalues for the same class of solvable potentials. In this approach, exact eigenvalues have been obtained by means of some phase distortions of WKB functions caused by the potential singularities in the complex plane. The needed phase distortions have been found with the use of quasiclassical asymptotics of exact solutions.
The question of exactness of the WKB approximation is usually reduced to the estimation of the high-order correction terms. The earliest development of the WKB method for obtaining the high-order corrections has been considered in Ref. [6]. Then, in [8], the radial generalization of Dunham’s one-dimensional WKB quantization condition was derived with the help of the Langer transformation [7]. It was shown that the second- and third-order integrals identically vanish for the hydrogen atom and the three-dimensional harmonic oscillator [8].

One method (see, for example, Ref. [12]) simply compares the modified WKB result with the eigenvalues obtained from an exact solution of the Schrödinger equation. A second method (as in [8]) proceeds by showing that all additional high-order correction terms to the WKB integral vanish for the given potential [8]. These proofs, however, are not entirely rigorous since these correction terms are only asymptotically valid, i.e., as \( \hbar \to 0 \) [10]. Furthermore, in the cases when a modified WKB integral gives the exact eigenvalues, it is not even clear which ”correction” must be shown to be zero. Thus a different approach is necessary if we are to prove the exactness of the leading-order WKB quantization condition.

In this work we develop an approach to show the exactness of the semiclassical approximation. We show that exact eigenvalues for the class of solvable potentials can be reproduced by the usual leading-order WKB quantization rule without any modification of the method. Our approach to the problem under consideration differs essentially from known ones [4],[6]-[12], where the one-dimensional problems have been considered. Unlike the previous approaches, instead of modification of the WKB method, we analyze an original three-dimensional equation and begin our analysis from the classic problem in the Hamilton-Jacobi formulation.

We analyze the semiclassical approximation in quantum mechanics using two basic principles: the correspondence principle and the adiabatic one. Starting from the three-dimensional classic problem and using the two principles mentioned above, we derive a wave equation appropriate in the quasiclassical region. This ”semiclassical” wave equation has canonical form, i.e., it does not contain first derivatives. Solving this equation for the spherically symmetric potentials by the usual (to leading order in \( \hbar \)) WKB method, we obtain exact energy eigenvalues for all spherically symmetric potentials. The corresponding eigenfunctions have the same form as the asymptotes of the exact solutions.

2. WKB approximation for the radial equation

Let us consider the Schrödinger equation for a spherically symmetric potential \( V(r) \),

\[
(-i\hbar)^2 \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] \psi(\vec{r}) = 2m[E-V(r)]\psi(\vec{r}).
\]

(1)

If one substitutes \( \psi(\vec{r}) = [U(r)/r]Y_{lm}(\theta, \varphi) \) into Eq. (1), one obtains (after separation) the one-dimensional problem for an effective potential \( V_{eff}(r) = V(r) + [l(l+1)\hbar^2/2mr^2] \):

\[
\left[ \frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \left( E - V(r) - \frac{l(l+1)\hbar^2}{2mr^2} \right) \right] U(r) = 0.
\]

(2)
For the two-turning-point problems, the standard leading-order WKB quantization condition is [13]

$$\int_{x_1}^{x_2} \sqrt{p^2(x)} dx = \pi \hbar \left( n + \frac{1}{2} \right), \quad n = 0, 1, 2, \ldots,$$

(3)

where $x_1, x_2$ are the classical turning points, $p^2(x) = 2m[E - V(x)]$, and $V(x)$ is the potential. Application of the quantization condition (3) to the radial equation (2) for the solvable spherically symmetric potentials does not reproduce the exact energy spectrum for the solvable potentials.

There is another difficulty arising in the semiclassical consideration of the radial Schrödinger equation (2). This equation has no the centrifugal term when $l = 0$. This means that (i) the effective potential $V_{\text{eff}}(r) = V(r) + \left[ l(l+1)\hbar^2/2mr^2 \right]$ has no (for example, the Coulomb potential) minimum, (ii) the problem has no left turning point and, as a result, (iii) we can not calculate the ground state because we can not use the WKB quantization condition (3) derived for two-turning-point problems.

In addition, the WKB solution of the radial Schrödinger equation is irregular at $r \to 0$, i.e., $R_{\text{WKB}}(r) \propto r^\lambda/\sqrt{r}$, $\lambda = \sqrt{l(l+1)}$, whereas the exact solution in this limit is $R(r) \propto r^l$. In order for the first-order WKB approximation to give the exact eigenvalues, the quantity $l(l+1)$ in Eq. (2) must be replaced by $(l + \frac{1}{2})^2$ [7].

The reason for this modification for the special case of the Coulomb potential was pointed out in Ref. [7] from the Langer transformation

$$r = e^x, \quad U(r) = e^{x/2}X(x),$$

(4)

which mapped the point $r = 0$ (for the radial problem) onto $x = -\infty$ (for the one-dimensional one) and $r \to \infty$ into $x \to \infty$ [8]. As a result of such a transformation the wave function $X(x)$ of the one-dimensional problem approaches zero for $x \to \pm\infty$, whereas the radial part of the solution $R(r)$ approaches zero for $r \to 0$ and $\infty$. The effective potential obtained when (4) is substituted into Eq. (2) takes the form

$$V_{\text{eff}}(r) = V(r) + \frac{(l + \frac{1}{2})^2\hbar^2}{2mr^2}.$$  

(5)

The second- and third-order WKB corrections to the energy quantization condition, derived in Ref. [8], have been shown to be identically zero for the Coulomb potential. These corrections are zero also for the harmonic oscillator. However, for other spherically symmetric potentials, in order to obtain the appropriate Langer-like correction terms, another special transformation of the wave function and its arguments are required.

In the general case of spherically symmetric potentials, the practical use shows that the quantization rule (3) for the effective potential (5) yields in many cases exact energy eigenvalues. In addition, the replacement $l(l+1) \to (l + \frac{1}{2})^2$ regularizes the radial WKB wave function at the origin and ensures correct asymptotic behavior at large quantum numbers.

In actual applications, the Langer correction in the radial Schrödinger equation (2) is usually used without any proof [14]-[16]. Meanwhile, this correction has a deep physical origin. In this work we give a foundation to the Langer replacement and show the existence
(in the quasiclassical region) of an integral of motion, $\vec{M}^2 = (l + \frac{1}{2})^2 \hbar^2$. Our approach results in an effective potential of the form (5), ensures the correct behavior of the WKB wave function at $r \to 0$, and provides its correct asymptotic behavior. The quantization condition (3) gives the exact energy spectrum.

In Ref. [12], exact eigenvalues for several potentials have been obtained with the help of some phase distortions of WKB functions caused by the potential singularities in the complex plane. Herein, in Ref. [12], as in the case of Langer transformation, the needed phase distortion is the "quarter". In fact, this additional constant $\frac{1}{4}$ changes (as will be shown below) the constant of motion $\vec{L}^2 = l(l+1)\hbar^2$ by $\vec{M}^2 = (l + \frac{1}{2})^2 \hbar^2$. Therefore, the phase distortion and Langer correction require the same modification of the WKB solution, namely, the changing squared angular momentum eigenvalues.

The WKB solution of the angular Schrödinger equation has, analogous to the radial solution, incorrect behavior at $\theta \to 0$: $\Theta_{WKB}(\theta) \propto \theta^\mu$, $\mu^2 = m^2 - \frac{\hbar^2}{4}$, while the exact regular solution in this limit is $\Theta_{r}^m(\theta) \propto \theta^{|m|}$. Therefore the angular equation also should be modified in the quasiclassical region to have for the function $\Theta_{WKB}^m(\theta)$ the same behavior at $\theta \to 0$ as the exact one.

In this paper we show that the main problem concerning the exactness of the WKB approximation is to reduce the Schrödinger equation to the "correct" canonical form, i.e., to the equation without first derivatives. In the case of the spherical coordinates, the Langer transformation changes the centrifugal term $l(l+1)\hbar^2/r^2$ in the Schrödinger equation by $(l + \frac{1}{2})^2 \hbar^2/r^2$. In fact, this requires changing the equation of motion in the quasiclassical region. The required form of the wave equation and, as a result, the centrifugal term can be obtained within the framework of the same semiclassical approach. Below we deduce the so-called semiclassical wave equation that has the necessary canonical form.

3. Semiclassical wave equation

One of the fundamental principles of quantum mechanics is the correspondence principle, which has been used at the stage of the creation of the quantum theory. The WKB method is the mathematical realization of the correspondence principle and it is usually used as a tool to obtain the approximate solution of the one-dimensional Schrödinger equation in the quasiclassical region at large values of quantum numbers. However, this same principle is used to derive the wave equation in quantum mechanics.

Consider the classical problem in the Hamilton-Jacobi formulation. The static Hamilton-Jacobi equation for a particle of mass $m$ moving in the field of the spherically symmetric potential $V(r)$ is

$$
\left( \frac{\partial S_0}{\partial r} \right)^2 + \frac{1}{r^2} \left( \frac{\partial S_0}{\partial \theta} \right)^2 + \frac{1}{r^2 \sin^2 \theta} \left( \frac{\partial S_0}{\partial \varphi} \right)^2 = 2m [E - V(r)] ,
$$
(6)

where $S_0$ is the classical action of the system. The wave equation in quantum mechanics can be obtained with the use of the classical equation according to the correspondence principle: $f \to \hat{f}$, where $f$ is the physical quantity and $\hat{f}$ is the corresponding operator.

Let us write the equation corresponding to (6) in a quantum mechanical form as
\[ \left( \hat{p}^2_r + \hat{p}^2_\theta + \frac{\hat{p}^2_\varphi}{r^2 \sin^2 \theta} \right) \tilde{\psi}(\vec{r}) = [E - V(r)] \tilde{\psi}(\vec{r}), \]  

(7)

where \( \hat{p}_q \) is the operator of the momentum conjugated with the coordinate \( q \) (\( q = r, \theta, \varphi \) for the spherical coordinates). To find the apparent form of the operators \( \hat{p}^2_q \), let us represent the function \( \tilde{\psi}(\vec{r}) \) in the form

\[ \tilde{\psi}(\vec{r}) = A \exp \left[ \frac{i}{\hbar} S(\vec{r}) \right], \]

(8)

where \( S(\vec{r}) \) is the action in quantum mechanics and \( A \) is the arbitrary constant. Consider the second derivatives of the function \( \tilde{\psi}(\vec{r}) \). For the second derivative \( \partial^2 \tilde{\psi}/\partial r^2 \) we have:

\[ \frac{\partial^2 \tilde{\psi}}{\partial r^2} = \left[ \left( \frac{i}{\hbar} \frac{\partial S}{\partial r} \right)^2 + \frac{i}{\hbar} \frac{\partial^2 S}{\partial r^2} \right] \tilde{\psi}, \]

or

\[ \left( -i\hbar \frac{\partial}{\partial r} \right)^2 \tilde{\psi} = \left[ \left( \frac{\partial S}{\partial r} \right)^2 + \hbar \frac{\partial^2 S}{\partial r^2} \right] \tilde{\psi}. \]

(9)

Now, according to the WKB method, substitute into (9) the expansion of the action \( S(\vec{r}) \) in powers of \( \hbar \), \( S(\vec{r}) = S_0(\vec{r}) + \hbar S_1(\vec{r}) + \hbar^2 S_2(\vec{r}) + ... \). Then we obtain to leading order in \( \hbar \),

\[ \left( -i\hbar \frac{\partial}{\partial r} \right)^2 \tilde{\psi} \simeq \left( \frac{\partial S_0}{\partial r} \right)^2 \tilde{\psi}. \]

(10)

Equation (10) is appropriate in the quasiclassical region where the following condition is satisfied:

\[ \left( \frac{\partial S_0}{\partial r} \right)^2 \gg \hbar \left| \frac{\partial^2 S_0}{\partial r^2} \right|. \]

(11)

By definition, the value \( p_r = \partial S_0 / \partial r \) is the radial momentum. Therefore the corresponding operator on the left-hand side of Eq. (10) is the squared radial momentum operator, i.e.,

\[ \hat{p}^2_r = \left( -i\hbar \frac{\partial}{\partial r} \right)^2. \]

(12)

The form of the operators \( \hat{p}^2_\theta, \hat{p}^2_\varphi \) is found analogously:

\[ \hat{p}^2_\theta = \left( -i\hbar \frac{\partial}{\partial \theta} \right)^2, \quad \hat{p}^2_\varphi = \left( -i\hbar \frac{\partial}{\partial \varphi} \right)^2, \]

(13)

and Eq. (7) takes the form:

\[ (-i\hbar)^2 \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] \tilde{\psi}(\vec{r}) = 2m [E - V(r)] \tilde{\psi}(\vec{r}). \]

(14)
Equation (14) is the second-order differential equation in canonical form. This semi-classical wave equation is closely related to the classical one (6) and is appropriate to describe quantum systems in the quasiclassical region. It is easy to see that Eq. (14) can be obtained from the classical Hamilton-Jacobi equation (6) with the help of the correspondence principle

\[ \frac{\partial S_0}{\partial q} \rightarrow -i\hbar \frac{\partial}{\partial q}, \quad q = r, \theta, \phi. \]  

As will be demonstrated below, Eq. (14) is solved by the WKB method in the elementary functions and the corresponding energy eigenvalues coincide with the exact ones for the many solvable potentials. The correlation of the function \( \tilde{\psi}(\vec{r}) \) with the wave function \( \psi(\vec{r}) \) in the Schrödinger Eq. (1) is given by

\[ \tilde{\psi}(\vec{r}) = \sqrt{\det g_{ij}} \psi(\vec{r}), \]  

which follows from the identity: \( \int |\psi(\vec{r})|^2 d^3\vec{r} \equiv \int |\tilde{\psi}(\vec{r})|^2 \det g_{ij} dr d\theta d\phi = 1 \), where \( g_{ij} \) is the metric tensor (\( \det g_{ij} = r^2 \sin \theta \) for the spherical coordinates).

4. Semiclassical quantization in examples

As is well known, working within the framework of the usual WKB approximation, one does not get the exact spectrum from the leading-order term for many solvable potentials such as Hulthén and Rosen-Morse potentials unless one supplements it with Langer-like correction terms that are different for different potentials. However, application of the leading-order WKB quantization rule (3) to the semiclassical Eq. (14) gives, as one can easily check, the exact energy eigenvalues for all solvable spherically symmetric potentials and no further Langer-like corrections are necessary.

To illustrate Eq. (14) consider several classic problems. For the spherically symmetric potentials Eq. (14) is separated, yielding three second-order equations

\[ \left( -i\hbar \frac{d}{dr} \right)^2 \tilde{R}(r) = \left[ 2m \left( E - V(r) \right) - \frac{\tilde{M}^2}{r^2} \right] \tilde{R}(r), \]  

\[ \left( -i\hbar \frac{d}{d\theta} \right)^2 \tilde{\Theta}(\theta) = \left[ \tilde{M}^2 - \frac{M_z^2}{\sin^2 \theta} \right] \tilde{\Theta}(\theta), \]  

\[ \left( -i\hbar \frac{d}{d\phi} \right)^2 \tilde{\Phi}(\phi) = M_z^2 \tilde{\Phi}(\phi), \]  

where \( \tilde{M}^2, M_z^2 \) are the constants of separation and, at the same time, integrals of motion. The squared angular momentum \( \tilde{L}^2 \) defined from the Schrödinger equation, takes the values \( \tilde{L}^2 = l(l + 1) \hbar^2 \). In this section we show that, in the quasiclassical region, the squared angular momentum takes other values, namely \( \tilde{M}^2 = (l + \frac{1}{2})^2 \hbar^2 \).
A. Angular momentum in the quasiclassical region

The WKB quantization rule has proven to find approximate eigenvalues for the one-dimensional or radial Schrödinger equation. As for the angular Schrödinger equation, the WKB quantization rule does not reproduce exact eigenvalues. Besides, as mentioned above, the WKB solution of the angular Schrödinger equation, \( \Theta^{WKB}(\theta) \), has incorrect behavior at \( \theta \rightarrow 0 \) and \( \pi \).

Let us deal with the angular Eqs. (18) and (19), which determine the angular momentum and its projection in the quasiclassical region. Equation (19) determines eigenvalues of the angular momentum projection operator \( \vec{M}^2_\nu = [-i\hbar(d/d\varphi)]^2 \). The solution of this equation, \( \Phi_m(\varphi) \), is well known: \( \Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, M_z = m\hbar, m = 0, \pm 1, \pm 2, \ldots \).

Equation (18) is especially important in our semiclassical approach since it determines the squared angular momentum eigenvalues \( \vec{M}^2 \) that enter into the radial equation (17). The WKB quantization condition (3) appropriate to Eq. (18) and the WKB solution at the interval \([\theta_1, \theta_2] \)

\[
\int_{\theta_1}^{\theta_2} \sqrt{p^2(\theta)} d\theta = \pi \hbar \left( n_\theta + \frac{1}{2} \right), \quad n_\theta = 0, 1, 2, \ldots, \tag{20}
\]

\[
\Theta^{WKB}(\theta) = \frac{A}{\sqrt{|p(\theta)|}} \cos \left( \int_{\theta_1}^{\theta} \sqrt{p^2(\theta)} d\theta - \frac{\pi}{4} \right), \tag{21}
\]

where \( p^2(\theta) = \vec{M}^2 - M^2_\nu / \sin^2 \theta \); \( \theta_1, \theta_2 \) are the roots (classical turning points) of the equation \( p^2(\theta) = 0 \) and \( A \) is the arbitrary constant. Introducing a variable \( \alpha = \theta - \frac{\pi}{2} \) the phase integral (20) can be written in closed form

\[
\sqrt{\vec{M}^2 - M^2_\nu} \int_{\alpha_1}^{\alpha_2} \sqrt{1 - k^2 \sin^2 \alpha} \frac{d\alpha}{\cos \alpha} = \pi \left( \sqrt{\vec{M}^2} - \sqrt{M^2_\nu} \right),
\]

where \( k^2 = \vec{M}^2 / (\vec{M}^2 - M^2_\nu) \). Setting \( M_z = m\hbar \), we get, for the \( \vec{M}^2 \),

\[
\vec{M}^2 = \left( l + \frac{1}{2} \right)^2 \hbar^2, \quad l = |m| + n_\theta. \tag{22}
\]

Equation (22) represents the squared angular momentum eigenvalues in the quasiclassical region. Since the eigenvalues (22) have been obtained from the solution of the angular equation (18), this result is appropriate for any spherically symmetric potential. As noted above, the WKB solution \( \Theta^{WKB}(\theta) \) of the angular Schrödinger equation has incorrect asymptotes at \( \theta \rightarrow 0 \) and \( \pi \). At the same time, the WKB solution (21) corresponding to the eigenvalues (22) has the correct asymptotic behavior at these points for all values of \( l \).

So far, as the momentum \( p(\theta) \simeq |m| / \theta \) at \( \theta \rightarrow 0 \), this gives, for the WKB solution in the representation of the wave function \( \psi(\vec{r}) \) (see Eq. (16)), \( \Theta^{WKB}(\theta) = \Theta^{WKB}(\theta) / \sqrt{\sin \theta} \propto \theta^{|m|} \) which corresponds to the behavior of the exact wave function \( Y_{lm}(\theta, \varphi) \) at \( \theta \rightarrow 0 \). The normalized quasiclassical solution (21) far from the turning points, where \( p(\theta) \simeq (l + \frac{1}{2})\hbar \), has the form

\[
\tilde{\Theta}_l^m(\theta) = \sqrt{\frac{2}{\pi l - |m| + \frac{1}{2}}} \cos \left[ (l + \frac{1}{2}) \theta - \frac{\pi}{2} |m| - \frac{\pi}{4} \right], \tag{23}
\]
which, for the function $\Theta_l^m(\theta)$, agrees with the asymptote of the spherical functions $Y_{lm}(\theta, \varphi)$.

Now, using the obtained solution of the angular semiclassical Eq. (18), let us consider the radial Eq. (17). Substituting (22) into Eq. (17), we obtain the radial semiclassical equation for the effective potential (5) and no further Langer-like correction is necessary. The leading-order WKB quantization condition (3) appropriate to the radial Eq. (17) is

$$\int_{r_1}^{r_2} \sqrt{p^2(r)dr} = \pi \hbar \left(n_r + \frac{1}{2}\right), \quad n_r = 0, 1, 2, \ldots, \quad (24)$$

where the classical turning points $r_1, r_2$ are roots of the equation

$$p^2(r) \equiv 2m[E - V(r)] - \frac{(l + \frac{1}{2})^2\hbar^2}{r^2} = 0. \quad (25)$$

It is easy to check that the quantization condition (24) yields exact energy eigenvalues for all solvable spherically symmetric potentials $V(r)$, such as the Coulomb potential, the three-dimensional harmonic oscillator, and other ones. To demonstrate Eq. (14), let us consider several potentials of interest.

B. The Morse potential, $V(r) = V_0[e^{2\alpha(r-r_0)} - 2 \ e^{-\alpha(r/r_0-1)}]$

For this potential, let us consider, first, the radial Schrödinger equation (2), which does not contain the centrifugal term at $l = 0$:

$$\left(-i\hbar \frac{d}{dr}\right)^2 U(r) = 2m \left[E - V_0 e^{-2\alpha(r-r_0)/r_0} + 2V_0 e^{-\alpha(r-r_0)/r_0}\right] U(r) = 0. \quad (26)$$

The first-order WKB quantization condition appropriate to this equation is

$$\int_{r_1}^{r_2} \sqrt{2m[E - V_0 e^{-2\alpha(r-r_0)/r_0} + 2V_0 e^{-\alpha(r-r_0)/r_0}]dr} = \pi \hbar (n_r + \frac{1}{2}). \quad (27)$$

Introducing a variable $x = e^{-\alpha(r-r_0)/r_0}$, we reduce the phase-space integral to the well-known one. The sequential simple calculations result in the exact energy eigenvalues

$$E_n = -V_0 \left[1 - \frac{\alpha \hbar (n_r + \frac{1}{2})}{r_0 \sqrt{2mV_0}}\right]^2. \quad (28)$$

Now, let us deal with the semiclassical equation (17) for this potential, which (unlike the Schrödinger equation) contains the non-vanishing centrifugal term $[\hbar^2/4r^2]$ at $l = 0$:

$$\left(-i\hbar \frac{d}{dr}\right)^2 \tilde{R}(r) = \left[2m \left(E - V_0 e^{-2\alpha(r-r_0)/r_0} + 2V_0 e^{-\alpha(r-r_0)/r_0}\right) - \frac{(l + \frac{1}{2})^2\hbar^2}{r^2}\right] \tilde{R}(r) = 0. \quad (29)$$

The WKB quantization condition (24) appropriate to Eq. (29) is:

$$I = \int_{r_1}^{r_2} \sqrt{2m \left(E - V_0 e^{-2\alpha(r-r_0)/r_0} + 2V_0 e^{-\alpha(r-r_0)/r_0}\right) - \frac{\lambda^2}{r^2}}dr = \pi (n' + \frac{1}{2}), \quad (30)$$
where $\lambda = \hbar (l + \frac{1}{2})$. In the region $r > 0$, the problem under consideration has two turning points $r_1, r_2$ which are defined by Eq. (25). To calculate this integral introduce the variable $\rho = \frac{r}{r_0}$ and replace the integral along the interval $[\rho_1, \rho_2]$ by the contour integral in the complex plane $\rho$ with $\text{Re} \rho = \frac{r}{r_0}$, where the integral is taken about a contour $C$ enclosing the classical turning points $\rho_1, \rho_2$ and there are no other singularities of $\rho(r)$. Now, using the method of stereographic projection, we should exclude the singularities outside the contour $C$, i.e., at $\rho = 0$ and $\infty$. Excluding these infinities we have, for the integral (30),

$$I = \frac{1}{2} \oint \sqrt{2mr_0^2[E - V_0 e^{-2\alpha(r-1)} + 2V_0 e^{-\alpha(r-1)}]} \frac{-\lambda^2}{\rho^2} d\rho = \frac{1}{2}(I_1 + I_2), \quad (31)$$

where

$$I_1 = r_0 \sqrt{2m} \oint_{C_1} \sqrt{E - V_0 e^{-2\alpha(r-1)}} + 2V_0 e^{-\alpha(r-1)} d\rho$$

is reduced to the integral considered above and $I_2 = \oint_{C_2} \sqrt{-\lambda^2/\rho^2} d\rho = -2\pi \lambda$.

Therefore for the phase-space integral (31) we have

$$I = -\pi \lambda - \frac{\pi r_0}{\alpha} \left( \sqrt{-2mE} - \sqrt{2mV_0} \right) \quad (32)$$

and for the energy eigenvalues this gives

$$E_n = -V_0 \left[ 1 - \alpha \frac{h(n_r + \frac{1}{2}) + \lambda}{r_0 \sqrt{2mV_0}} \right]^2. \quad (33)$$

Setting in (33) $\lambda = 0$, we arrive at the formula (28) obtained from the Schrödinger equation at $l = 0$. However, in our case $\lambda_{\text{min}} = \hbar/2$ at $l = 0$ and the energy eigenvalues are:

$$E_n = -V_0 \left[ 1 - \alpha \frac{\hbar(n_r + 1)}{r_0 \sqrt{2mV_0}} \right]^2. \quad (34)$$

Formula (34) for $E_n$ is different from the expression (28) obtained from the Schrödinger equation for the Morse potential at $l = 0$. This difference is caused by the centrifugal term $[\hbar^2/4r^2]$ in the radial semiclassical Eq. (17) at $l = 0$. Thus we obtain two results for the Morse potential by the WKB method: the known exact eigenvalues (28) obtained from the Schrödinger equation and another result (34) obtained from solution of Eq. (17).

### C. The Hulthén potential, $V(r) = -V_0 e^{-r/r_0} / (1 - e^{-r/r_0})$

The Hulthén potential is known as nonsolvable by the standard WKB method potentials, unless one supplements it with Langer-like corrections. However, solving the semiclassical equation (14) for this potential by the usual WKB method, we obtain the exact analytic result.

The leading-order quantization condition (24) for the Hulthén potential is

$$I = \int_{r_1}^{r_2} \sqrt{2m \left( E + V_0 e^{-r/r_0} \right) - \frac{(l + \frac{1}{2})^2 \hbar^2}{r^2}} dr = \pi \hbar (n' + \frac{1}{2}). \quad (35)$$
In the region $r > 0$, this problem has two turning points $r_1, r_2$. The phase-space integral (35) is calculated analogously to the above case. Replace the integral along the interval $[r_1, r_2]$ by the contour integral in the complex plane of the variable $\rho$, $\rho = \frac{r}{r_0}$, where contour $C$ encloses the classical turning points $\rho_1, \rho_2$. Using the method of stereographic projection, we should exclude the infinities outside the contour $C$. Excluding these infinities we have, for (35),

$$I = \frac{1}{2} \oint C \sqrt{2mr_0^2 \left( E + V_0 \frac{e^{-\rho}}{1 - e^{-\rho}} \right) - \frac{(l + \frac{1}{2})^2 h^2}{\rho^2}} d\rho = \frac{1}{2}(I_1 + I_2),$$

(36)

where

$$I_1 = \oint_{C_1} \sqrt{2mr_0^2 \left( E + V_0 \frac{e^{-\rho}}{1 - e^{-\rho}} \right)} d\rho,$$

and $I_2 = i\hbar (l + \frac{1}{2}) \oint_{C_2} \frac{d\rho}{\rho}$.

To calculate the integral $I_1$, let us introduce the variable $z = e^\rho - 1$. Then the simple integration gives, for $I_1$,

$$I_1 = r_0 \sqrt{2m} \oint_{C_2} \frac{dz}{\sqrt{E + \frac{V_0}{z} \frac{dz}{z + 1}}} \equiv$$

$$r_0 \sqrt{2m} \left( \oint_{C_{\infty}} \sqrt{E + \frac{V_0}{z} \frac{dz}{z + 1}} - \oint_{C_{-1}} \sqrt{Ez^2 + V_0z} \frac{dz}{z + 1} \right) =$$

$$2\pi r_0 \sqrt{-2m} \left[ -\sqrt{-E} + \sqrt{-E+V_0} \right].$$

Substituting the integration result into Eq. (35), we immediately get the exact energy spectrum

$$E_n = -\frac{1}{8mr_0^2} \left( \frac{2mV_0r_0^2}{N} - N \right)^2,$$

(38)

where $N = (n' + l + 1)\hbar$ denotes the principal quantum number.

Thus application of the standard leading-order WKB approximation to the wave Eq. (14) yields the exact energy eigenvalues for the solvable spherically symmetric potentials. In our approach, the radial equation (17) has the centrifugal term $(l + \frac{1}{2})^2 h^2/\ell^2$ for any spherically symmetric potential $V(r)$ because the squared angular momentum eigenvalues $\vec{M}^2 = (l + \frac{1}{2})^2 h^2$ are obtained in a natural way from solution of the angular semiclassical equation (18) with the use of the same WKB method. In other words, we have shown that the Langer replacement $l(l+1) \rightarrow (l + \frac{1}{2})^2$ requires the modification of the angular momentum. This correction is universal for any spherically symmetric potential and no further corrections are necessary.
5. Generalization and discussion

The standard lowest-order WKB prescription reproduces the exact energy levels for the one-dimensional harmonic oscillator and three-dimensional harmonic oscillator in the Cartesian coordinates \(x, y, z\). But just these two problems are correctly formulated in the framework of the semiclassical approach: in the Cartesian coordinates \(x, y, z\), the Schrödinger equation has the required canonical form and coincides with the semiclassical one.

The required canonical form is (in the spherical coordinates) the semiclassical Eq. (14), in which the centrifugal term has the form \((l + \frac{1}{2})^2 \hbar^2 / r^2\) for all spherically symmetric potentials. An analogous semiclassical wave equation can be written in the general case of the curvilinear coordinates \(q_1(x, y, z)\), \(q_2(x, y, z)\), \(q_3(x, y, z)\):

\[
\left[ \sum_{k=1}^{3} \left( -i \hbar \frac{\partial}{\partial q_k} \right)^2 \right] \tilde{\psi}(\vec{q}) = 2m \left[ E - V(r) \right] \tilde{\psi}(\vec{q}),
\]

(39)

where \(g_{kk}\) are the elements of the metric tensor. The correlation of the function \(\tilde{\psi}(\vec{q})\) with the wave function \(\psi(\vec{q})\) of the Schrödinger equation is given by the formula (16). The quasiclassical condition (11) implies that the momentum \(\partial S_0 / \partial r\) is large enough, i.e., the quantum number \(n\) takes large values. At the same time, the WKB method yields exact eigenvalues for all values of \(n\). To disentangle this contradiction let us return to Eq. (9) and show that the condition (11) can be generalized.

In Eq. (9), the expression in the square brackets has a sense of squared momentum. In order for the operator \([(-i\hbar)\partial/\partial r]^2\) to be Hermitian this expression should be real. This is possible if \(\partial^2 S_0 / \partial r^2 \approx 0\). What does this condition mean? This implies the adiabatically slow alteration of the derivative \(\partial S_0 / \partial r\), i.e.,

\[
\frac{\partial S_0}{\partial r} \approx \text{const.}
\]

(40)

Unlike the condition (11), the constraint (40) supplies the hermiticity of the operator (12) and does not imply that the momentum \(\partial S_0 / \partial r\) takes large values. Further, this constraint anticipates the final result, i.e., discrete constant eigenvalues \(k_n\) of the operator (12). Integrating (40), we obtain, for the action \(S_0(r)\), \(S_0(r) = p_n r + \text{const.}\) where \(p_n\) is the momentum expressed via the energy eigenvalue \(E_n\), \(p_n = \sqrt{2m |E_n|}\), and the final solution can be written in elementary functions. In the region of the classical motion, where \(p(r) > 0\), this solution has the form of a standing wave

\[
\tilde{R}_n(r) = A \cos \left( \frac{p_n r}{\hbar} - \chi_1 - \frac{\pi}{4} \right),
\]

(41)

where \(\chi_1\) is the value of the phase integral (24) at the turning point \(r_1\). Analogous solutions can be written for other one-dimensional equations obtained after separation of Eq. (14). These solutions are in agreement with the asymptotic solutions of the corresponding exact solutions of the Schrödinger equation (1).
6. Conclusion

In conclusion, let us summarize the results obtained. Our approach to the problem under consideration is different from known ones [4], [6]-[12] in which the one-dimensional or radial problems have been considered. In this work, we have considered an approach concerning the application of the WKB method to the three-dimensional problems in quantum mechanics. Whereas previous workers were considering modification of the WKB method or were using some transformations of the one-dimensional equations obtained after separation, we start with the original three-dimensional problem. We have shown that the main problem is to reduce the Schrödinger equation to the correct canonical form, i.e., to an equation without first derivatives.

The main result of this work is the derivation of the semiclassical wave Eq. (14) [or in general form (39)] appropriate in the quasiclassical region; to do this, the basic principles of quantum mechanics were used: the correspondence principle and the adiabatic one. Unlike the Schrödinger equation (1), the semiclassical one (14) results in another integral of motion, i.e., the squared angular momentum \( \vec{M}^2 = (l + \frac{1}{2})^2 \hbar^2 \). This means that the centrifugal term in the radial equation (17) has the form \((l + \frac{1}{2})^2 \hbar^2 / r^2\) for any spherically symmetric potential \(V(r)\). It is important to emphasize that the squared angular momentum eigenvalues \(\vec{M}^2 = (l + \frac{1}{2})^2 \hbar^2\) have been obtained in our approach in a natural way from the solution of the angular semiclassical equation (18) in the framework of the same WKB method. In other words, we have obtained the justification of the Langer correction as the correction to the squared angular momentum eigenvalues.

We have shown that the solution of the obtained wave equation (14) by the standard WKB method (to leading order in \(\hbar\)) gives the exact eigenvalues for all solvable spherically symmetric potentials. The corresponding eigenfunctions have the same behaviour as the asymptotes of the exact solutions. A generalization of the semiclassical equation for the arbitrary curvilinear coordinates \(q_1(x, y, z), q_2(x, y, z), q_3(x, y, z)\) has been obtained.

We have considered here the three-dimensional problem in spherical coordinates. To deal with the one-dimensional or other multi-dimensional problems, one must, first of all, write the equation under consideration in the correct canonical form. For this one should start from the corresponding classical Hamilton-Jacobi equation and, using the correspondence principle (15), write a wave equation. Then each of the one-dimensional equations obtained after separation is solved by the WKB method.

Thus the standard leading-order WKB approximation is the appropriate method to solve the semiclassical wave equation (14) obtained. We have shown that quantization, the apparent form of the operators, and many results of quantum mechanics (exact eigenvalues, correct asymptotic behaviour of the semiclassical wave functions at the origin and at infinity, and the correct phases of the WKB solutions) can be obtained within the framework of the standard semiclassical approach.

Acknowledgment. This work was supported in part by the Belarusian Fund for Fundamental Researches.
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