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Wkb Solutions for Inversely Quadratic Yukawa plus Inversely Quadratic Hellmann Potential

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Abstract: The exact energy spectrum for inversely quadratic Yukawa plus potential plus inversely quadratic Hellmann potential was obtained, via the WKB approach. Also three special cases of the potential have been considered and their energy eigenvalues obtained.

Keywords: Schrodinger Equation, Inversely Quadratic Yukawa Potential, Inversely Quadratic Hellmann, WKB Approximation

1. Introduction

One of the earliest and simplest methods of obtaining approximate eigenvalues of the one-dimensional Schrodinger equation in the limiting case of large quantum numbers was originally proposed by Wentzel, Kramers, and Brillouin known as the WKB approximation method [1]. The Wentzel-Kramers-Brillouin (WKB) Approximation was first introduced in quantum mechanics in 1926, although it had been developed earlier. This approximation is important since at the beginning of the development of quantum mechanics, physicists around the world were attempting to solve the Schrodinger and Schrodinger-like equations. In 1928 Gamow used the Approximation to theoretically describe alpha decay for the first time [2]. In the lowest- order approximation, the WKB quantization condition is

$$\int_{r_1}^{r_2} \sqrt{2m\big(E - V(r)\big)}\, dr = \pi\hbar \left(n + \tfrac{1}{2}\right), n = 0, 1, 2 \qquad (1)$$

In general, Equation (1) yields moderately accurate eigenvalues as analytic functions of the parameters contained in the potential. An exact analytical solution of Schrodinger equation for central potentials has attracted tremendous interest in recent years. Example of these potentials are the parabolic type potential [3], the Eckart potential [4, 5], the Fermi-step potential [4, 3], the Rosen-Morse potential [6], the Ginocchio barrier [7], the Scarf barriers [6], the Morse potential [8] and a potential which interpolates between Morse and Eckart barriers [8]. To properly use the WKB approximation for a three dimensional problem with spherical symmetry, one has to apply the one-dimensional WKB formalism to the radial Schrodinger equation

$$\frac{\partial^2 \Psi}{\partial r^2} + \frac{2m}{\hbar^2}\left[E - V_{eff}(r)\right]\Psi = 0 \qquad (2)$$

where the effective potential $V_{eff}(r)$ is

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

Such a straightforward application leads to an important difficulty in obtaining exact energy eigen value solution because the WKB reduced radial wave function at the origin has a behaviour which is different from that of the true wave function [2]. For this reason, Langer [5] suggested that the strength of the angular momentum should be treated as an adjustable parameter K, not as a fixed quantity. Langer pointed out that K should be replaced with the term $\left(l+\frac{1}{2}\right)^2$ in the lowest order quantization formula which has great physical meaning. The replacement of $l(l+1) \rightarrow \left(l+\frac{1}{2}\right)^2$ regularizes the radial WKB wave function at the origin and ensure correct asymptotic behaviour at large quantum numbers.

The aim of this work is to solve the Schrodinger equation for the inversely quadratic Yukawa plus inversely quadratic Hellmann (IQYIQH) potential via the WKB approximation method. The IQYIQH takes the form:

$$V(r) = -\frac{V_0}{r^2}e^{-2\alpha r} - \frac{V_1}{r} + \frac{V_2}{r^2}e^{-\alpha r} \tag{3}$$

where α is the screening parameter and $V_0, V_1 \& V_2$ are the depths of the potential. Recently, Ita*et al* [9] have used a form of the potential known as a class of the Yukawa potential plus Manning-Rosen potential to obtain bound state solution of the SE via NU Method. The IQH potential was first studied in a mixed form with the Mie type potential in 2013 by Itaand co-workers [10, 11, 12, 13] where they obtain the solution of the Schrodinger equation via NU method. Also, analytical expressions for the bound state of the inversely quadratic Hellmann plus inversely quadratic potential has been reported by Ita *et al* [14-16]. Not much has been done in solving the IQYIQH potential via the WKB method. This paper therefore seeks to address this issue and is organized as follows; Section 1 has the introduction, a brief description of the semiclassical quantization and the WKB approximation for the radial solution is reviewed in section 2. In section 3, the radial Schrodinger equation with IQYIQH potential was solved, followed by a brief discussion in section 4, and finally, conclusion in section 5

2. Semiclassical Quantization and the WKB Approximation

In this section, quasiclassical solution of the Schrodinger's equation for the spherically symmetric potentials was considered. Given the Schrodinger equation for a spherically symmetric potentials $V(r)$ of equation (3) as

$$(-i\hbar)^2\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right)\psi(r,\theta,\phi) = \left[2m\left(E - V(r)\right)\right]\psi(r,\theta,\phi) \tag{4}$$

The total wave function in eq. (3) can be defined as

$$\psi(r,\theta,\phi) = [rR(r)]\left[\sqrt{sin\theta}\,\Theta(\theta)\Phi(\phi)\right] \tag{5}$$

And by decomposing the spherical wave function in equation (4) using equation (5), the following equations were obtained:

$$\left(-i\hbar\frac{\mathrm{d}}{\mathrm{dr}}\right)^2 R(r) = \left[2m\left(E - V(r)\right) - \frac{\vec{M}^2}{r^2}\right]R(r) \tag{6}$$

$$\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}\theta}\right)^2 \Theta(\theta) = \left[\vec{M}^2 - \frac{M_z^2}{\sin^2\theta}\right]\Theta(\theta) \tag{7}$$

$$\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}\phi}\right)^2 \Phi(\phi) = M_z^2\Phi(\phi) \tag{8}$$

Where $\vec{M}^2$, M_z^2 are the constants of separation and, at the same time, integrals of motion. The squared angular momentum $\vec{M}^2 = \left(l+\frac{1}{2}\right)^2\hbar^2$.

Considering equation (6), the leading order WKB quantization condition appropriate to equation (3) is

$$\int_{r_1}^{r_2}\sqrt{P^2(r)}\,dr = \pi\hbar\left(n+\frac{1}{2}\right),\ \mathrm{n} = 0, 1, 2... \tag{9}$$

where $r_2 \& r_1$ are the classical turning point known as the roots of the equation

$$P^2(r) = 2m\left(E - V(r)\right) - \frac{\left(l+\frac{1}{2}\right)^2\hbar^2}{r^2} = 0 \tag{10}$$

equation (9) is the WKB quantization condition which is subject for discussion in the preceding section. Consider Eq. (6)-(8) in the framework of the quasiclassical method, the solution of each of these equations in the leading $\hbar$ approximation can be written in the form

$$\Psi^{WKB}(r) = \frac{A}{\sqrt{P(r,\lambda)}}exp\left[\pm\frac{i}{\hbar}\int\sqrt{P^2(r)}\,dr\right] \tag{11}$$

3. Solutions to the Radial Schrödinger Equation

The radial Schrodinger equation for the IQYIQH potential can be solved approximately using the WKB quantization condition equation (9). Since the potential of interest slowly varies, we assume that the wave function remains sinusoidal. Hence, the effective potential was used and plugged it in to the WKB approximation of equation (10) and to obtain the exact solution, we consider two turning points.

Given the effective potential with the centrifugal term as

$$V_{eff}(r) = -\frac{V_0}{r^2}e^{-2\alpha r} - \frac{V_1}{r} + \frac{V_2}{r^2}e^{-\alpha r} + \frac{\left(l+\frac{1}{2}\right)^2\hbar^2}{2mr^2} \tag{12}$$

where α is the screening parameter and $V_0, V_1 \& V_2$ are the depths of the potential.

The potential in equation (12) can also be written in the form

$$V_{eff}(r) = \frac{(V_2 - V_0)}{r^2} + \frac{(2V_0\alpha - V_1 - V_2\alpha)}{r} + (V_2\alpha^2 - 2V_0\alpha^2) + \frac{\left(l+\frac{1}{2}\right)^2\hbar^2}{2mr^2} \tag{13}$$

Substitute equatin (13) into equation (9), we have

$$\int_{r_1}^{r_2}\sqrt{P^2(r)}\,dr=\int_{r_1}^{r_2}\sqrt{2m\left(E-\frac{(V_2-V_0)}{r^2}-\frac{(2V_0\alpha-V_1-V_2\alpha)}{r}-(V_2\alpha^2-2V_0\alpha^2)-\frac{\left(l+\frac{1}{2}\right)^2\hbar^2}{2mr^2}\right)}\,dr=\pi\hbar\left(n+\frac{1}{2}\right) \quad (14)$$

let $\vec{M}^2=\left(l+\frac{1}{2}\right)^2\hbar^2$

$$\int_{r_1}^{r_2}\sqrt{2m\left(E-\frac{(V_2-V_0)}{r^2}-\frac{(2V_0\alpha-V_1-V_2\alpha)}{r}-(V_2\alpha^2-2V_0\alpha^2)-\frac{\vec{M}^2}{2mr^2}\right)}\,dr=\pi\hbar\left(n+\frac{1}{2}\right) \quad (15)$$

Factoring $\frac{1}{r^2}$ and $\sqrt{2m}$, we have

$$\sqrt{2m}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{\left((E+2V_0\alpha^2-V_2\alpha^2)r^2-(2V_0\alpha-V_1-V_2\alpha)r-\left(\frac{2m(V_2-V_0)-\vec{M}^2}{2m}\right)\right)}\,dr=\pi\hbar\left(n+\frac{1}{2}\right) \quad (16)$$

if $(E+2V_0\alpha^2-V_2\alpha^2)=-\tilde{E}$ and factoring out $\tilde{E}$, we obtain

$$\sqrt{2m\tilde{E}}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{\left(-r^2-\frac{(2V_0\alpha-V_1-V_2\alpha)}{\tilde{E}}r-\left(\frac{2m(V_2-V_0)-\vec{M}^2}{2m\tilde{E}}\right)\right)}\,dr=\pi\hbar\left(n+\frac{1}{2}\right) \quad (17)$$

let $-\frac{(2V_0\alpha-V_1-V_2\alpha)}{\tilde{E}}=B$, and $\left(\frac{2m(V_2-V_0)-\vec{M}^2}{2m\tilde{E}}\right)=C$, we have

$$\sqrt{2m\tilde{E}}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{(-r^2+Br-C)}\,dr=\pi\hbar\left(n+\frac{1}{2}\right) \quad (18)$$

$$\sqrt{2m\tilde{E}}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{(r-r_1)(r_2-r)}\,dr=\pi\hbar\left(n+\frac{1}{2}\right) \quad (19)$$

Wherewe obtain the turning points $r_2\&r_1$ from the terms inside the square roots as

$$r_1=\frac{-B-\sqrt{B^2-4C}}{2}$$

$$r_2=\frac{-B+\sqrt{B^2-4C}}{2}$$

Solving the integral of equation (19) explicitly, we obtain

$$\sqrt{2m\tilde{E}}\left(-\frac{(2V_0\alpha-V_1-V_2\alpha)}{\tilde{E}}-2\sqrt{\left(\frac{2m(V_2-V_0)-\vec{M}^2}{2m\tilde{E}}\right)}\right)=2\hbar\left(n+\frac{1}{2}\right) \quad (20)$$

$$\tilde{E}=\frac{2m(2V_0\alpha-V_1-V_2\alpha)^2}{\left(\hbar\left(n+\frac{1}{2}\right)+\sqrt{\left(2m(V_2-V_0)+\vec{M}^2\right)}\right)^2} \quad (21)$$

$$E=V_2\alpha^2-2V_0\alpha^2-\frac{m(V_1+V_2\alpha-2V_0\alpha)^2/2\hbar^2}{\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+\frac{2m}{\hbar^2}(V_2-V_0)}\right)^2} \quad (22)$$

4. Discussion

Having obtained the energy eigen values (equation 22) and corresponding eigen functions of the IQYIQH potential, it's seen that the WKB approximation method is general for all types of problems in quantum mechanics, simple from the physical point of view, and its correct application results in the exact energy eigenvalues for all solvable potentials. We now consider the following cases of the potential

Case 1. If we set the parameters $V_0=V_2=0$, $V_1=\frac{e^2}{4\pi\epsilon_0}$, it is easy to show that equation (22) reduces to the bound state energy spectrum of a particle in the Coulomb potential

$$E^{c}{}_{n,l}=-\frac{m\left(\frac{e^2}{4\pi\epsilon_0}\right)^2/2\hbar^2}{(n+l+1)^2} \quad (23)$$

$$E^{c}{}_{n,l}=-\frac{me^4}{32\hbar^2\pi^2\epsilon_0{}^2n_p{}^2} \quad (24)$$

$$n_p=n+l+1 \quad (25)$$

Case 2: If we set the parameter $-V_0=B, -2V_0\alpha=A, -2V_0\alpha^2=C$, $V_1=V_2=0$ in equation (13), it is easy to show that equation (22) reduces to the bound state energy spectrum of a vibrating-rotating diatomic molecule subject to the mie type potential as follows

$$E^{M}{}_{n,l}=C-\frac{mA^2/2\hbar^2}{\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+\frac{2m}{\hbar^2}B}\right)^2} \quad (26)$$

Case 3: If we set the parameters $C = 0$, in the energy expression of equation (26), it is easy to show that equation (26) reduces to the bound state energy spectrum of kratzer-Feus potential as follows

$$E^{KF}{}_{n,l} = C - \frac{mA^2/2\hbar^2}{\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+\frac{2m}{\hbar^2}B}\right)^2} \tag{27}$$

Case 4: If we set the parameters $V_1 = V_0 = 0$, in the energy expression of equation (22), we obtain the bound state energy spectrum of inversely quadratic effective potential as

$$E^{IQE}{}_{n,l} = V_2\alpha^2 - \frac{m(V_2\alpha)^2/2\hbar^2}{\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+\frac{2m}{\hbar^2}V_2}\right)^2} \tag{28}$$

Case 5: If we set the parameters $V_0 = 0$, in the energy expression of equation (22), we obtain the bound state energy spectrum of inversely quadratic Hellmann potential as

$$E^{IQH}{}_{n,l} = V_2\alpha^2 - \frac{m(V_1+V_2\alpha)^2/2\hbar^2}{\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+\frac{2m}{\hbar^2}(V_2-V_0)}\right)^2} \tag{29}$$

Case 6: If we set the parameters $V_1 = 0, V_2 = -V_2$ in the energy expression of equation (22), we obtain the bound state energy spectrum of a class of Yukawa potential as

$$E = -V_2\alpha^2 - 2V_0\alpha^2 - \frac{m(V_2\alpha+2V_0\alpha)^2/2\hbar^2}{\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2-\frac{2m}{\hbar^2}(V_2+V_0)}\right)^2} \tag{30}$$

5. Conclusion

The WKB Approximation has been studied and applied to Inversely Quadratic Yukawa and Inversely Quadratic Hellmann Potential. Although the WKB approximation is a quite rough numerical calculation, however our results can be applied to spectroscopic analysis of diatomic molecules.

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