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Solution of the Schrödinger equation with inversely quadratic Yukawa potential (IQYP) plus Kratzer-Fues (KFP) potential using the WKB quantum mechanical formalism

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ABSTRACT: The main objective of this research work is theoretical investigate the bound state solutions of the non-relativistic Schrödinger equation with a mixed potential composed of the Inversely Quadratic Yukawa/Attractive Coulomb potential plus a Modified Kratzer potential (IQYCKFP) by utilizing the Wentzel-Kramers-Brillouin (WKB) quantum theoretical formalism. The energy eigenvalues and its associated wave functions have successfully been obtained in sequel to certain diatomic molecules includes; HCL, HBr, LiH.

Bound State Solution of the Schrödinger Equation

$$E_{ne} = D_e - 2V_0\delta^2 - \frac{m(A + 2D_e r_e - 2V_0\delta)^2 / 2\hbar^2}{\left[\left(n + \frac{1}{2}\right) + \sqrt{\left(\ell + \frac{1}{2}\right)^2 - \frac{2m}{\hbar^2}\left(V_0 - D_e r_e^2\right)}\right]^2}$$

1. Introduction

One of the interesting problems in quantum mechanics is to get exact solutions of the Schrödinger equation. To do this, a real potential is often selected to serve as the driving force of the energy eigenvalues and the eigenfunctions of the Schrödinger equation[1-3]. These state solutions reveal the particle dynamics in non-relativistic quantum mechanics[2]. Numerous researchers have investigated the bound states of the Schrödinger equation using variety of potentials and quantum formalism. Some of these potentials play critical roles in many fields of Physics such as Molecular Physics, Solid State and Chemical Physics[4]. The Manning-Rosen potential has been studied in-depth and have also been utilized in quantum systems and Yukawa potential, and its classes have been studied in Schrödinger formalism[5,6].

In this work, using the Wentzel, Kramers and Brillouin (WKB) quantum approximation, we shall investigate the bound state solutions of the Schrödinger equation using a combination of potentials known as the Inversely Quadratic Yukawa/Attractive Coulomb potential plus a Modified Kratzer potential (IQYCKFP).

2. The WKB Theoretical Approximation

In this section, we consider the quasiclassical solution of the Schrödinger's equation for the spherically symmetric potentials. Given the Schrödinger equation for a spherically symmetric potentials $V(r)$ of Equation 3 as

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

The total wave function in Equation 3 can be defined as

$$\psi(r,\theta,\phi) = [rR(r)]\left[\sqrt{sin\theta}\,\Theta(\theta)\Phi(\phi)\right] \quad (2)$$

And by decomposing the spherical wave function in Equation 1 using Equation 2 we obtain the following equations:

$$\left(-i\hbar\frac{\mathrm{d}}{\mathrm{dr}}\right)^2 R(r) = \left[2m\big(E - V(r)\big) - \frac{\vec{M}^2}{r^2}\right] R(r), \quad (3)$$

$$\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}\theta}\right)^2 \Theta(\theta) = \left[\vec{M}^2 - \frac{M_z^2}{\sin^2\theta}\right] \Theta(\theta), \quad (4)$$

$$\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}\phi}\right)^2 \Phi(\phi) = M_z^2\Phi(\phi) \quad (5)$$

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

$$\int_{r_1}^{r_2} \sqrt{P^2(r)}\, dr = \pi\hbar\left(n + \frac{1}{2}\right), \text{ n=0, 1, 2} \quad (6)$$

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

$$P^2(r) = 2m\big(E - V(r)\big) - \frac{\left(l+\frac{1}{2}\right)^2\hbar^2}{r^2} = 0 \quad (7)$$

Equation 9 is the WKB quantization condition which is subject for discussion in the preceding section. Consider Equations 5-7 in the framework of the quasi-classical method, the solution of each of these equations in the leading $\hbar$ approximation can be written in the form

$$\Psi^{WKB}(r) = \frac{A}{\sqrt{P(r,\lambda)}} exp\left[\pm\frac{i}{\hbar}\int \sqrt{P^2(r)}\, dr\right] \quad (8)$$

3. Solutions of the Schrödinger Equation

The Wentzel, Kramers and Brillouin surmise has been of tremendous importance to physicist, chemist, mathematician as regards quantum mechanics in view of the fact that it gives approximate solutions to linear differential equations. The inversely quadratic Yukawa/attractive Coulomb plus Kratzer Fues potential can be expressed thus

$$V(r) = -\frac{1}{r^2}(V_0) + \frac{1}{r}(2V_0\delta - A) + (-2V_0)\delta^2 \text{ and } V(r) = D_e\left(\frac{r - r_e}{r}\right)^2 \quad (9)$$

The sum of these potentials can be written as

$$V(r) = \frac{2V_0\delta}{r} - \frac{A}{r} - \frac{V_0}{r^2} - 2V_0\delta^2 + D_e - \frac{2D_e r_e}{r} + \frac{D_e r_e^2}{r^2} \quad (10)$$

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$$V_{eff\,(r)} = D_e - 2V_0\delta^2 + \frac{2V_0\delta}{r} - \frac{A}{r} - \frac{2D_e r_e}{r} - \frac{V_0}{r^2} + \frac{D_e r_e^2}{r^2} + \frac{\ell(\ell+1)\hbar^2}{2mr^2} \tag{11}$$

$$Q(r) = \sqrt{2m(E - V_{eff\,(r)})} \tag{12a}$$

Equation 12a stands for the classical formula for momentum.

$$\int_{ra}^{rb} Q(r)dr = \left(n + \tfrac{1}{2}\right)\pi\hbar;\ \text{n=0, 1,2,3…} \tag{12b}$$

Upon, substituting Equations 11 and 12a into 12b i.e. the (WKB) we have

$$\int_{ra}^{rb} \sqrt{2m\left(E_{ne} - D_e + 2V_0\delta^2 - \frac{2V_0\delta}{r} + \frac{A}{r} + \frac{2D_e r_e}{r} + \frac{V_0}{r^2} - \frac{D_e r_e^2}{r^2} - \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right)}dr = \left(n + \tfrac{1}{2}\right)\pi\hbar$$

Factoring out $\sqrt{2m}$ (13)

$$\sqrt{2m}\int_{rA}^{rB} \sqrt{\left(E_{ne} - D_e + 2V_0\delta^2 - \frac{2V_0\delta}{r} + \frac{A}{r} + \frac{2D_e r_e}{r} + \frac{V_0}{r^2} - \frac{D_e r_e^2}{r^2} - \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right)}dr = \left(n + \tfrac{1}{2}\right)\pi\hbar \tag{14}$$

$$\sqrt{2m}\int_{rA}^{rB} \sqrt{\frac{1}{r^2}\left[\left(E_{ne} - D_e + 2V_0\delta^2\right)r^2 + \left(-2V_0\delta + A + 2D_e r_e\right)r - \left(D_e r_e^2 - V_0 + \frac{\ell(\ell+1)\hbar^2}{2m}\right)\right]}dr$$
$$= n + \tfrac{1}{2}\pi\hbar \tag{15}$$

$$\sqrt{2m}\int_{rA}^{rB} \frac{1}{r}\sqrt{\left[\left(E_{ne} + 2V_0\delta^2 - D_e\right)r^2 + \left(A + 2D_e r_e - 2V_0\delta\right)r - \left(D_e r_e^2 - V_0 + \frac{\ell(\ell+1)\hbar^2}{2m}\right)\right]}dr$$
$$= \left(n + \tfrac{1}{2}\right)\pi\hbar \tag{16}$$

$$\left.\begin{aligned} -A &= E_{ne} + 2V_0\delta^2 - D_e \\ M &= A + 2D_e r_e - 2V_0\delta \\ N &= D_e r_e^2 - V_0 + \frac{\ell(\ell+1)\hbar^2}{2m} \end{aligned}\right\}$$
where the negative sign on -(A) indicates a bound state.

Upon substituting the representations made into Equation 16 we have

$$\sqrt{2m}\int_{ra}^{rb} \frac{1}{r}\left(\sqrt{-\tilde{A}r^2 + Mr - N}\right)dr = \left(n + \tfrac{1}{2}\right)\pi\hbar. \tag{17}$$

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Factoring out $\sqrt{\tilde{A}}$, we have

$$\sqrt{2m\tilde{A}}\int_{ra}^{rb}\frac{1}{r}\left(\sqrt{-r^2+\frac{M}{\tilde{A}}r-\frac{N}{\tilde{A}}}\right)dr=\left(n+\tfrac{1}{2}\right)\pi\hbar. \tag{18}$$

x represent $\frac{M}{\tilde{A}}$ and y as $\frac{N}{\tilde{A}}$

$$\sqrt{2m\tilde{A}}\int_{ra}^{rb}\frac{1}{r}\left(\sqrt{-r^2+xr-y}\right)dr=\left(n+\tfrac{1}{2}\right)\pi\hbar. \tag{19}$$

$$\sqrt{2m\tilde{A}}\int_{ra}^{rb}\frac{1}{r}\sqrt{(r-r_a)(r_b-r)}dr=\left(n+\tfrac{1}{2}\right)\pi\hbar. \tag{20}$$

Where we obtain the classical turning points r_a and r_b from the terms inside the square roots as;

$$r_a=\frac{x-\sqrt{x^2-4y}}{2},\ r_b=\frac{x+\sqrt{x^2-4y}}{2} \qquad \text{N/N: }\begin{Bmatrix} r_a+r_b=x \\ r_ar_b=y \end{Bmatrix} \tag{21}$$

Recall

$$\int_{r_a}^{r_b}\frac{1}{r}\sqrt{(r-r_a)(r_b-r)}dr=\pi\left[\frac{1}{2}(r_a+r_b)-\sqrt{r_ar_b}\right] \tag{22}$$

$$\sqrt{2m\tilde{A}}\cdot\frac{\pi}{2}\left(x-2\sqrt{y}\right)=\left(n+\tfrac{1}{2}\right)\pi\hbar \tag{23}$$

$$\tilde{A}=\frac{2mM^2}{4\left[\hbar\left(n+\tfrac{1}{2}\right)+\sqrt{2mN}\right]^2} \tag{24}$$

Upon substituting the coefficients of M, N, $\tilde{A}$ *into* Equation 24 to obtain the energy eigenvalue.

$$-E_{ne}-2V_0\delta^2+D_e=\frac{2m(A+2D_er_e-2V_0\delta)^2}{4\left[\hbar\left(n+\tfrac{1}{2}\right)+\hbar\sqrt{\frac{2mD_er_e^2-2mV_0}{\hbar^2}+\ell(\ell+1)}\right]^2} \tag{25a}$$

Initiating the Langer correction term $\ell\left(\ell+1\right)\to\left(\ell+\tfrac{1}{2}\right)^2$

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$$E_{ne} = D_e - 2V_0\delta^2 - \frac{m(A+2D_e r_e - 2V_0\delta)^2 \big/ 2\hbar^2}{\left[\left(n+\tfrac{1}{2}\right)+\sqrt{\left(\ell+\tfrac{1}{2}\right)^2 - \frac{2m}{\hbar^2}\left(V_0 - D_e r_e^2\right)}\right]^2} \tag{25b}$$

The above equation results in the bound state energy spectrum with respect to quantum numbers of a vibrating-rotating diatomic molecule subject to the (IQYCKFP) potential. Thus, its corresponding wave function is given as

$$R_{ne(r)} = N_{ne} r^{\left(-\frac{1}{2}+\sqrt{\left(\ell+\frac{1}{2}\right)^2+\frac{2m}{\hbar^2}(D_e r_e^2 - V_0)}\right)} e^{-r^2\left(\sqrt{\frac{m}{2\hbar^2}(D_e - E_{ne} - 2V_0\delta^2)}\right)}$$
$$F_1\left(-n; 1+\sqrt{\left(\ell+\tfrac{1}{2}\right)^2+\frac{2m}{\hbar^2}\left(D_e r_e^2 - V_0\right)};\ \left(2\sqrt{\frac{m}{2\hbar^2}\left(D_e - E_{ne} - 2V_0\delta^2\right)}\right) r^2\right) \tag{26}$$

4. Discussion

Having obtained the Energy Eigen Value and its corresponding (ψ) using the WKB approach for the Schrödinger equation with the (IQYCKFP), we understood that if we set up parameters $D_e = 0,\ V_0 \neq 0$ and $A = Ze^2$

$$E_{ne} = -2V_0\delta^2 - \frac{m(A-2V_0\delta)^2 \big/ 2\hbar^2}{\left[n+\tfrac{1}{2}+\sqrt{\left(\ell+\tfrac{1}{2}\right)^2 - \frac{2m}{\hbar^2}V_0}\right]^2} \tag{27}$$

5. Conclusions

It is much easy to show that Equation 19 has resulted to a bound state energy spectrum of a vibrating rotating diatomic molecule subject to the inversely quadratic Yukawa plus attractive coulomb potential.

Similarly, if $D_e \neq 0,\ V_0 = 0$ and $A \neq Ze^2 = 0$

$$E_{ne} = D_e - \frac{m(2D_e r_e)^2 \big/ 2\hbar^2}{\left[\left(n+\tfrac{1}{2}\right)+\sqrt{\left(\ell+\tfrac{1}{2}\right)^2 + \frac{2m}{\hbar^2}\left(D_e r_e^2\right)}\right]^2} \tag{28}$$

Equation 28 results to a bound state energy spectrum subject to Kratzer Fues potential.

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