ANALYSIS

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Discovery

Solutions of the Schrödinger Equation for the Superposed Screened Coulomb plus Kratzer Fues Potential Using the WKB Approximation Method

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The solutions of the Schrödinger equation with the Superposed Screened Coulomb plus Kratzer Fues (SSCKF) potential have been presented using the Wentzel Kramers Brillouin (WKB) approach. The bound state energy eigenvalue was obtained as;

$$E_{n1} = D_e + g_1\delta + 2g_2\delta - \frac{m(g_1 + g_2 + 2D_e r_e)^2 / 2\hbar^2}{\left[\left(n+\frac{1}{2}\right) + \sqrt{\left(l+\frac{1}{2}\right) + \frac{2mD_e r_e}{\hbar^2}}\right]^2}$$

Where negative energy eigenvalue indicates a bound state system. Also, particular case of this potential has been considered and their energy eigenvalue obtained.

INTRODUCTION

The WKB approximation was introduced in quantum mechanics in 1926 although had earlier development named after Wentzel, Kramers, and Brillouin. Generally, it's a method for finding approximate solutions to linear differential equations with spatially varying coefficients. In quantum mechanics, it is used to obtained approximate solutions to the time-independent one-dimensional Schrödinger equation. This approach (WKB) has been of vital importance as seen from the quantum mechanics point of view wherein several Physicist around the world were attempting to solve the Schrödinger and Schrödinger-like equations. Furthermore, a situation arising from the screened Coulomb potential is of indubitable importance in physics and Chemistry of atomic incidence. To address this situation, various methods have been applied both analytical and numerical. The method includes this research approach (WKB), etc.

In 2017 Ita et' al., used the approximation to theoretically describe the exact energy spectrum with the inversely quadratic Yukawa plus inversely quadratic Hellmann potential for the first time.

Consider the radial Schrödinger equation with the effective potential given as:

$$\frac{d^2R(r)}{dr^2} + \frac{2m}{\hbar^2}\left[E - Veff(r)\right]R(r) = 0 \quad (1) \qquad Veff(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2} \quad (2)$$

Also, the leading order WKB quantization condition is;

$$\int_{r_1}^{r_2} \sqrt{p_{(r)}^2}\, dr = \pi\hbar\left(n+\frac{1}{2}\right), n = 0,1,2,3 \quad (3)$$

Where r_1 and r_2 are the turning points of the potential.

$$P_{(r)}^2 = 2m\left(E - V_{(r)}\right)$$

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$P_{(r)} = \sqrt{2m(E - V_{(r)})}$ is the classical formula for momentum (4)

In 1937, Rodolph E. Langer suggested a correction $l(l+1) \rightarrow \left(l + \frac{1}{2}\right)^2$ which is known as Langer replacement or Langer correction. This arose because the range of the radial Schrödinger Equation is restricted from zero to infinity, as opposed to the entire real line. For 2D systems, the Langer correction goes $\left(l^2 - \frac{1}{4}\right) \rightarrow l^2$. The Langer correction is a correction when the WKB approximation method is applied to 3D problems with spherical symmetry. It can be described regarding a Maslov index for linear Lagrangian sub-manifolds. The goal of the present paper is to obtain solutions of the Schrödinger equation for the superposed Screened Coulomb Plus Kratzer Fues (SSCKF) potential using the WKB approximation method. The (SSCKF) is thus:

$$V_{(r)} = \frac{D_e (r - r_e)^2}{r^2} - \left(\frac{g_1 e^{-\delta r}}{r} + \frac{g_2 e^{-2\delta r}}{r} \right) \tag{5}$$

$$V_{(r)} = D_e - \frac{2D_e r_e}{r} + \frac{D_e r_e^2}{r^2} - \frac{g_1}{r} + g_1 \delta - \frac{g_2}{r} + 2g_2 \delta$$

Where g_1 and g_2 are coupling constants, D_e is the dissociation energy, δ the screening strength or parameter and r represents the internuclear distance. Equation (3) is then amenable to WKB method, to obtain the energy eigenvalue. Ita *et al.* have used a form of the potential known as a class of the Yukawa potential plus inversely quadratic Hellmann potential to obtain bound state solution of the Schrödinger Equation via the WKB approach. Bound state solution for quantum mechanical gravitational plus harmonic oscillator potential via the WKB method has been achieved by Louis et'al., 2017. Analytical solutions of Schrödinger equation for central potentials have gained tremendous interest in recent years. Examples of these potentials are the Rosen-Morse potential, Eckart potential, the Morse potential, Scarf barriers. By subjecting $g_1 = 0$ the modified screened Coulomb potential, as well as numerical calculations for the bound state, is obtained. Since the screened Coulomb potential plays a significant role in microscopic fields, this potential has been applied in different branches of atomic and molecular physics and chemistry. For this reason, Roy undertook studies on the critical parameters and spherical confinement of H atom in screened Coulomb potential using the GPS method. He extended his studies towards finding bound state energy Eigenvalues for the screened Coulomb potential and their corresponding wave functions as well as providing information's regarding sample dipole polarizability. Whereas this paper sought to offer solutions to problems arising in view and organized as follows; Section 1 has the introduction, and gives the WKB approximation for the radial solutions is reviewed. Section 2 provides the theoretical approach which defines a solution to the Schrödinger equation with (SSCKF) potential was solved, after that a brief discussion in section 3, lastly section 4 gives a conclusion.

SOLUTIONS TO THE SCHRÖDINGER EQUATION

The Schrödinger equation of the (SSCKF) potential can be solved approximately using the WKB quantization condition equation (3). Since the potential is quest slowly varies, we assume that the wave function remains sinusoidal. Hence the effective potential was used and plugged into the WKB approach of equation (4) and to obtain the exact solutions we consider some turning points. Given the effective potential with the centrifugal term as;

$$Veff\,(r) = D_e g_1 \delta + 2g_2 \delta - \frac{g_1}{r} - \frac{g_2}{r} - \frac{2D_e r_e}{r} + \frac{D_e r_e^2}{r^2} + \frac{l(l+1)\hbar^2}{2mr^2}$$

Langer; $l(l+1) = \left(l + \frac{1}{2}\right)^2$ (6)

Where δ is the screening strength and g_1, g_2 are coupling constants? D_e is the dissociation energy and r_e represents the equilibrium internuclear distance and $\frac{l(l+1)\hbar^2}{2mr^2}$ as the centrifugal term.

Substituting the effective potential into the classical formula for momentum

$$P(r)=\sqrt{2m(E-Veff\,(r))} \tag{7}$$

$$P(r)=\sqrt{2m\left(E-D_e-g_1\delta-2g_2\delta+\frac{g_1}{r}+\frac{g_2}{r}+\frac{2D_er_e}{r}-\frac{D_er_e^2}{r^2}-\frac{l(l+1)\hbar^2}{2mr^2}\right)} \tag{8}$$

Substitution equation (8) into (3) we have;

$$\int_{r_1}^{r_2}\sqrt{2m\left(\left[E_{n1}-D_e-g_1\delta-2g_2\delta\right]+\left[\frac{g_1}{r}+\frac{g_2}{r}+\frac{2D_er_e}{r}\right]-\left[\frac{D_er_e^2}{r^2}+\frac{l(l+1)\hbar^2}{2mr^2}\right]\right)}dr=\left(n+\tfrac{1}{2}\right)\pi\hbar \tag{9}$$

Factoring out $\sqrt{2m}$

$$\sqrt{2m}\int_{r_1}^{r_2}\sqrt{\left(\left[E_{n1}-D_e-g_1\delta-2g_2\delta\right]+\left[\frac{g_1}{r}+\frac{g_2}{r}+\frac{2D_er_e}{r}\right]-\left[\frac{D_er_e^2}{r^2}+\frac{l(l+1)\hbar^2}{2mr^2}\right]\right)}dr=\left(n+\tfrac{1}{2}\right)\pi\hbar \tag{10}$$

$$\sqrt{2m}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{\left(\left[E_{n1}-D_e-g_1\delta-2g_2\delta\right]r^2+\left[g_1+g_2+2D_er_e\right]r-\left[D_er_e^2-\frac{l(l+1)\hbar^2}{2m}\right]\right)}dr=\left(n+\tfrac{1}{2}\right)\pi\hbar \tag{11}$$

$$E_{ni}-D_e-g_1\delta-2g_2\delta=-\tilde{E}$$

$$g_1+g_2+2D_er_e=B$$

$$\frac{2mD_er_e^2+l(l+1)\hbar^2}{2m}=C$$

$$\sqrt{2m}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{-\tilde{E}r^2+Br-C}\,dr=\left(n+\tfrac{1}{2}\right)\pi\hbar \tag{12}$$

Factoring out $\sqrt{\tilde{E}}$ we have;

$$\sqrt{2m\tilde{E}}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{-r^2+\frac{Br}{\tilde{E}}-\frac{C}{\tilde{E}}}\,dr=\left(n+\tfrac{1}{2}\right)\pi\hbar \tag{13}$$

Let P represent $\frac{B}{\tilde{E}}$ and q as $\frac{C}{\tilde{E}}$

$$\sqrt{2m\tilde{E}}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{(-r^2+pr-q)}\ dr=\left(n+\tfrac{1}{2}\right)\pi\hbar \qquad (14)$$

$$\sqrt{2m\tilde{E}}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{(r-r_1)(r_2-r)}\ dr=\left(n+\tfrac{1}{2}\right)\pi\hbar \qquad (15)$$

Where we obtain the turning point r_1 & r_2 from the terms inside the squared roots as

$$r_1=\frac{p-\sqrt{p^2-4q}}{2}$$

$$r_2=\frac{p+\sqrt{p^2-4q}}{2}$$

Solving, explicitly the integral of equation (14), we obtain;

$$\sqrt{2m\tilde{E}}\cdot\frac{\pi}{2}\left(p-2\sqrt{q}\right)=\left(n+\tfrac{1}{2}\right)\pi\hbar \qquad (16)$$

$$\sqrt{2m\tilde{E}}\left(p-2\sqrt{q}\right)=2\left(n+\tfrac{1}{2}\right)\hbar \qquad (17)$$

Upon substituting the coefficients of p & q into equation (17) we obtain;

$$\sqrt{2m\tilde{E}}\left[\frac{B}{\tilde{E}}-\frac{2\sqrt{C}}{\sqrt{\tilde{E}}}\right]=2\hbar\left(n+\tfrac{1}{2}\right) \qquad (18)$$

$$\tilde{E}=\frac{2mB^2}{4\left[\hbar\left(n+\tfrac{1}{2}\right)+\sqrt{2mC}\right]^2} \qquad (19)$$

Upon substituting the coefficient of $\tilde{E}$ into equation (19) we have;

$$E_{nl}+D_e+g_1\delta+2g_2\delta=\frac{2mB^2}{4\left[\hbar\left(n+\tfrac{1}{2}\right)+\sqrt{2mC}\right]^2} \qquad (20)$$

$$E_{nl}=D_e+g_1\delta+2g_2\delta-\frac{m(g_1+g_2+2D_er_e)^2/2\hbar^2}{\left[\left(n+\tfrac{1}{2}\right)+\sqrt{\left(l+\tfrac{1}{2}\right)^2\frac{2mD_er_e^2}{\hbar^2}}\right]^2} \qquad (21)$$

Equation (21) results in the bound state energy spectrum subject to the superposed screened coulomb plus Kratzer Fues (SSCKF) potential.

DISCUSSION

In summary, we have obtained the energy eigenvalue using the Wentzel Kramers Brillouin (WKB) method for the Schrödinger equation with the superposed screened Coulomb plus Kratzer Fues potential. If we set parameters, $D_e = 0$ and $V(r) = \left[-g_1 e^{-\delta r} + g_2 e^{-2\delta r}\right]/r$, it's easy to show that equation (21) reduces to the bound state energy spectrum of a particle in the superposed screened Coulomb potential.

$$E_{nl} = \frac{-(g_1 + g_2)^2 m}{2\hbar^2 n_p{}^2} + g_1\delta + g_2\delta \quad (22)$$

Where $n_p = n + l + 1$ gives the principal quantum number.

Similarly, if we set $D_e \neq 0,\ V(r) = 0$ i.e $g_1 + g_2 = 0$ Equation (21) results in a bound state energy spectrum subject to the Kratzer Fues potential given as thus;

$$E_{nl} = D_e - \frac{m(2D_e r_e)^2 / 2\hbar^2}{\left[\left(n + \frac{1}{2}\right) + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2mD_e r_e^2}{\hbar^2}}\right]^2}$$

CONCLUSION

The bound state solutions of the Schrödinger equation have been obtained

$$D_e + g_1\delta + 2g_2\delta - \frac{m(g_1 + g_2 + 2D_e r_e)^2 / 2\hbar)}{\left[\left(n + \frac{1}{2}\right) + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2mD_e r_e^2}{\hbar^2}}\right]^2}$$

With the superposed screened Coulomb plus Kratzer Fues potential. Special cases of the potential considered and its energy eigenvalue obtained which is a satisfactory tool to the concepts of electromagnetic radiation and its interactions with matter.

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