Analysis of Ground State Energy Spectrum of Effective Hulthen Potential*

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Introduction

The radial Schrdinger equation is one of the most common equations in Mathematical physics. Its solution gives the probability amplitude of finding. It is known that the exact solution for Schrdinger equation is found only in few cases. The lack of explicit expression for eigenfunctions and the energy eigenstates in many cases in mainly due to the centrifugal term $\frac{1}{r^2}$ present in the equation. The use of Hulthen potential is good example to get rid of this problem. The Schrdinger Wave Equation can be solved exactly for only few cases of potential for all n and l.

The Hulthen potential is one of the important short-range potentials which behaves like a Coulomb potential for small values of r and decreases exponentially for large values of r. The Hulthen potential has received extensive study in both relativistic and non-relativistic quantum mechanics. However, the radial SWE for the Hulthen potential were exactly solvable for $l \neq 0$, analytically, but an exact wave function and energy eigen values are obtained at $l = 0$ using graphical method.

Theoretical Background

The Schrdinger wave equation is given by

$$\Big[-\frac{\hbar^2}{2m}\nabla^2 + V_H(r)\Big]\Psi(r) = E\Psi(r) \qquad (1)$$

The potential $V_H(r)$ is given by,

$$V_H(r) = -Ze^2\delta\frac{e^{-\delta r}}{1-e^{-\delta r}}, \qquad (2)$$

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where δ is the screening parameter and Z is a constant that is identified with the atomic number when the potential is used for the atomic phenomenon.

The radial part of SWE for the Hulthen potential is given by

$$\Big[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{2mE}{\hbar^2} + \frac{2m}{\hbar^2}Ze^2\delta\frac{e^{-\delta r}}{1-e^{-\delta r}} - \frac{l(l+1)}{r^2}\Big]\psi_n(r) = 0$$

Where $\psi_n(r) = rR(r)$

Where l is a constant responsible for separation of radial part of SWE from its angular part.

Using the D-dimensional polar coordinates with polar variable r (hyper radius) and the angular momentum variable $\theta_1, \theta_2, \theta_3, ...\theta_{D-2}, \phi$ (hyper angle), the Laplacian operator can be written as,

$$(\bigtriangledown_D)^2 = r^{1-D}\frac{\partial}{\partial r}\Big(r^{D-1}\frac{\partial}{\partial r}\Big) + \frac{(\Lambda_D)^2(\Omega)}{r^2} \qquad (3)$$

where $(\Lambda_D)^2(\Omega)$ is a partial differential operator on the unit sphere S^{D-1} (Laplace-Betrami operator or grand orbital operator) and it is defined analogously to a three-dimensional (3D) angular momentum as $(\Lambda_D)^2(\Omega) = -\Sigma_{i\geq j}^{D}(\Lambda_{ij}^2)$,where $\Lambda_{ij}^2 = x_i\frac{\partial}{\partial x_j} - x_j\frac{\partial}{\partial x_i}$ for all Cartesian components x_i of the D-dimensional vector $(x_1, x_2, x_3, ...x_D)$.

The D-dimensional Schroedinger equation has the form,

$$-\frac{\hbar^2}{2M}(\bigtriangledown_D)^2\Psi_{nlm}(r,\Omega) + V(r)\Psi_{nlm}(r,\Omega) = E\Psi_{nlm}(r,\Omega) \qquad (4)$$

The hyper radial equation for the Hulthen potential can be written as follows:

$$R_{nl}''(r)+\frac{D-1}{r}+\frac{l(l+D-2)}{r^2}R_{nl}(r)+\frac{2M}{\hbar^2}\left[E+Z\delta\frac{e^{-\delta r}}{1-e^{-\delta r}}\right]R_{nl}(r)=0 \quad (5)$$

where $R_{nl}(r)$ is the hyper-radial part of the wave-function, E is the energy eigenvalue, l is the orbital angular momentum quantum number and n_r is the hyper-radial quantum number. Equation (2.2.6) is called the D-dimensional hyper-radial Schrdinger equation for the Hulthen potential.

Eigenvalues of the Hulthen potential in D-dimensions can be solved using the Nikiforov-Uvarov method. If we define,

$$R_{nl}(r)=r^{-\frac{(D-1)}{2}}U_{nl}(r) \quad (6)$$

in above equation,

$$U''_{nl}(r)+\left[\frac{2M}{\hbar^2}\left(E+Z\delta\frac{e^{-\delta r}}{1-e^{-\delta r}}\right)-\frac{(2l+D-1)(2l+D-3)}{4r^2}\right]U_{nl}(r)=0 \quad (7)$$

The above equation is similar to the 1D Schrdinger equation for the Hulthen potential. We can extend the solution to a multidimensional case using the Nikiforov-Uvarov method to yield:

$$E_n{}^D=-\frac{1}{2}\left[\frac{2}{2n+D-3}-\left(\frac{2n+D-3}{4}\right)\delta\right]^2 \quad (8)$$

where n is the principal quantum number given as $n=n_r+l+1$. The critical screening parameter δ_c (for which $E_n=0$), can be obtained from equation as $\delta_c=8/(2n+D-3)^2$ for $D\geqslant 3$.

Results and Discussions

For a fixed value of angular momentum quantum number l, the energy spectrum increases as the principal quantum number n_r increases for a small screening parameter δ. As increase in angular momentum quantum number l, leads to an increase in the energy spectrum as the principle quantum number increases for a varying screening potential. In other words for a weak potential coupling strength, solutions are ignored due to the presence of imaginary terms and the energy spectrum is not complex but real. Beyond this, we can observe from the table, the energy eigenvalue is strongly bounded and an increase in rotational quantum number l makes the energy become attractive with increasing δ.

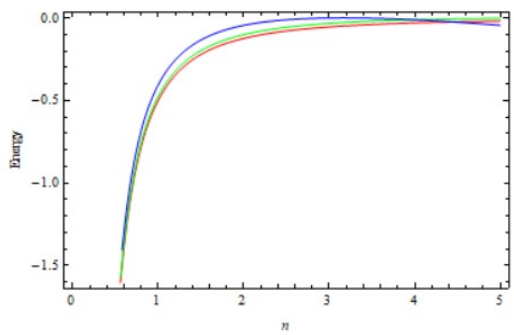

FIG. 1: Energy Spectrum [Red→ δ=0.02 , Green→ δ=0.05, Blue → δ=0.2]

The difference between various methods become more apparent for large values of δ parameters and appear due to the approximation of the centrifugal term, which simply means that the better the accuracy in calculating energy eigenvalues the better the approximation of the centrifugal term, and hence the whole model.

Acknowledgements

Two of us (APM and KBV) are grateful to VGST, Department of Science and Technology, Government of Karnataka, India for supporting our research (KSTePS/VGST-K-FIST L-1/2018-19/GRD NO.769).

References

[1] D Agboola 2009 Phys. Scr. 80 065304.
[2] S. M. Ikhdair, R. Sever, Ap- plied Mathematics and Computation 216 (3) (2010) 911923.
[3] Y. P. Varshni,Phys. Rev. A 41 (1990) 46824689.
[4] J. Stanek,Central European Journal of Chemistry 9 (2011) 737742
[5] W.-C. Qiang, Y. Gao, R.-S. Zhou,Journal of Physics 6 (2) (2008) 356362