International Research Journal of Pure and Applied Physics
Vol.6, No.1, pp.1-7, September 2019
Published by European Centre for Research Training and Development UK (www.eajournals.org)

BOUND-STATES SOLUTIONS OF THE RADIAL SCHRODINGER EQUATION FOR A GAUSSIAN POTENTIAL WITHIN THE FRAMEWORK OF THE NIKIFOROV-UVAROV METHOD

E. Omugbe[1], O.E. Osafile [2] And E.A Enaibe[2]

[1] Doctoral programme, Department of Physics, Federal University of Petroleum Resources, *P. M. B. 1221*, Effurun Delta State, Nigeria.
[2]Department of Physics, Federal University of Petroleum Resources, *P. M. B. 1221*, Effurun Delta State, Nigeria.

ABSTRACT: *In this paper, we studied the approximate bound-state solutions of the radial Schrodinger equation with a quantum mechanical Gaussian potential, by using the generalized parametric Nikiforov-Uvarov method. The energy spectrum and the corresponding wave function were obtained analytically in closed form. The computed eigenvalues for the ground state and first excited state for sufficiently large potential depths are in good agreement with the results obtained with other methods.*

KEYWORDS: Schrodinger equation, Gaussian potential, Nikiforov-Uvarov method.

INTRODUCTION

Starting from the Schrodinger equation (SE), the eigenvalues and wave-functions of quantum systems can be predicted. However, not all quantum systems are exactly soluble and as such the use of approximation methods and numerical schemes are required for determining the eigenstates of the system [1]. The SE with different quantum mechanical potentials have been discussed in the literature [2 – 8] .Hamzavi *et al.* [2] have calculated the bound state solutions of the SE for a Yukawa Potential by using the generalized parametric Nikiforov-Uvarov (NU) method. Ita et al. [3], used the Wentzel, Kramers, Brillouin, and Jeffery (WKBJ) approach to estimate the energy spectrum for the Manning-Rosen plus a class of Yukawa potential. Several methods [9 -14] have been applied to calculate the eigenvalues of the radial SE for an attractive Gaussian potential. The variational approximation approach [9, 10] and asymptotic Iteration method [11] were applied to calculate the bound state solutions of the SE for the quantum mechanical Gaussian potential (QMGP). The results of the variational method for sufficiently large potential depth reported in Refs. 9 and 10 are in good agreement with numerical solutions. Also, the Ricatti-Pade method [12] was used to find the eigenvalues of the QMGP for large potential depths, while Fernandez [13] applied the Wronskian method to find the exact energy spectrum of the Gaussian well for any potential well depth. To the best of our knowledge, the study of the eigensolutions within the framework of the NU method with a QMGP has not been reported. Therefore, the aim of this paper is to find an approximate analytical eigenvalue solution of the radial SE for an attractive QMGP by using the parametric NU method.

ISSN 2055-009X(Print), ISSN 2055-0103(Online)

RADIAL SCHRODINGER EQUATION

The three-dimensional time independent SE for a particle of mass m and wave-function $\psi(r,\theta,\phi)$ is given as

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

If we substitute $\psi(r,\theta,\phi)=\frac{R(r)Y(\theta,\phi)}{r}$ into Eq. (1), with the appropriate separation constant we obtained the radial equation as

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

where the last term in Eq. (2) is the centrifugal term with orbital quantum number l.

The quantum potential in Eq. (2) is a Gaussian well modeled as

$$V(r)=-V_0e^{-\alpha r^2} \quad (V_0,\ \alpha>0). \quad (3)$$

were V_0, and α are the well depth and screening parameter respectively.

In order to estimate the eigen-solutions of Eq. (2), we Taylor-expand the Gaussian function to get

$$V(r)=V_0(\alpha r^2-1). \quad (4)$$

It is worthwhile to mention that the truncated Gaussian potential in Eq. (4) is an accurate approximation owing to the fact that the Gaussian potential is a short-range potential which can be used in the study of a single particle motion in atomic nuclei and also in analyzing scanning tunneling microscope [10]

NIKIFOROV-UVAROV METHOD

The Nikiforov-Uvarov (NU) method is used to solve the second order differential equations with Special orthogonal polynomials [15]. The Schrodinger-type equation with the appropriate coordinate transformation $r\to s$ is given as

$$\psi_n''(s)+\frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s)=0, \quad (5)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of at most order 2 and $\tilde{\tau}(s)$ is of order 1.
Equation (5) for any quantum potential [16] has the general parametric form given as

$$\psi_n''(s)+\frac{(\lambda_1-\lambda_2 s)}{s(1-\lambda_3 s)}\psi_n'(s)+\frac{(-\gamma_1 s^2+\gamma_2 s-\gamma_3)}{s^2(1-\lambda_3 s)^2}\psi_n(s)=0. \quad (6)$$

The respective energy spectrums and eigen-functions equations [16] are given as

$$\lambda_2 n-\lambda_5(2n+1)+(2n+1)\left(\sqrt{\lambda_9}+\lambda_3\sqrt{\lambda_8}\right)+\lambda_3 n(n-1)+\lambda_7+2\lambda_3\lambda_8+2\sqrt{\lambda_8\lambda_9}=0, \quad (7)$$

ISSN 2055-009X(Print), ISSN 2055-0103(Online)

$$\psi_n(s) = N_n s^{\lambda_{12}}(1-\lambda_3 s)^{-\lambda_{12}-\frac{\lambda_{13}}{\lambda_3}} P_n^{\left(\lambda_{10}-1,\ \frac{\lambda_{11}}{\lambda_3}-\lambda_{10}-1\right)}(1-2\lambda_3 s), \tag{8}$$

where N_n and $P_n^{(\alpha,\beta)}$ are normalization constant and Jacobi polynomials respectively.

The parametric constants in Eq. (7) and Eq. (8) are given as

$$\lambda_4 = \frac{1}{2}(1-\lambda_1),\ \ \lambda_5 = \frac{1}{2}(\lambda_2 - 2\lambda_3),\ \ \lambda_6 = (\lambda_5)^2 + \gamma_1,\ \ \lambda_7 = 2\lambda_4\lambda_5 - \gamma_2,$$
$$\lambda_8 = (\lambda_4)^2 + \gamma_3,\ \ \lambda_9 = \lambda_3\lambda_7 + (\lambda_3)^2\lambda_8 + \lambda_6,\ \ \lambda_{10} = \lambda_1 + 2\lambda_4 + 2\sqrt{\lambda_8}\ , \tag{9}$$
$$\lambda_{11} = \lambda_2 - 2\lambda_5 + 2\left(\sqrt{\lambda_9} + \lambda_3\sqrt{\lambda_8}\right),\ \ \lambda_{12} = \lambda_4 + \sqrt{\lambda_8},\ \ \lambda_{13} = \lambda_5 - \left(\sqrt{\lambda_9} + \lambda_3\sqrt{\lambda_8}\right),$$

"In some problems" [16] λ_3=0 such that

$$\lim_{\lambda_3\to 0} P_n^{\left(\lambda_{10}-1,\ \frac{\lambda_{11}}{\lambda_3}-\lambda_{10}-1\right)}(1-\lambda_3 s) = L_n^{\lambda_{10}-1}(\lambda_{11}s), \tag{10}$$

and

$$\lim_{\lambda_3\to 0}(1-\lambda_3 s)^{-\lambda_{12}-\frac{\lambda_{13}}{\lambda_3}} = e^{\lambda_{13}s} \tag{11}$$

By substituting Eqs. (10) and (11) into Eq. (8), the wave function has the form given as

$$\psi_n(s) = s^{\lambda_{12}}\, e^{\lambda_{13}s}\ L_n^{\lambda_{10}-1}(\lambda_{11}s) \tag{12}$$

ENERGY SPECTRUM AND EIGEN-FUNCTION SOLUTIONS

To calculate the energy spectrums we write Eq. (2) with the approximate potential given in Eq. (4) as

$$\frac{d^2R(r)}{dr^2} + \frac{2m}{\hbar^2}\left[(E+V_0) - V_0\alpha r^2 - \frac{l(l+1)\hbar^2}{2mr^2}\right]R(r) = 0, \tag{13}$$

Using dimensionless variables

$$r = \rho\zeta,\quad \rho = \sqrt{\frac{\hbar}{V_0\alpha m}},\quad \epsilon = \frac{E+V_0}{\hbar V_0\alpha}, \tag{14}$$

with the following derivatives

$$\frac{dR(r)}{dr} = \frac{dR(r)}{d\zeta}\times\frac{d\zeta}{dr},\quad \frac{d^2R(r)}{dr^2} = \frac{1}{\rho^2}\frac{d^2R(r)}{d\zeta^2}, \tag{15}$$

We can rewrite Eq. (13) as

ISSN 2055-009X(Print), ISSN 2055-0103(Online)

$$\frac{d^2R(\zeta)}{d\zeta^2} + (2\epsilon - \frac{2}{\hbar}\rho^2\zeta^2 - \frac{l(l+1)}{\zeta^2})R(\zeta) = 0. \quad (16)$$

In order to put Eq. (16) into the form of Eq. (6), we set $\zeta^2 = s$ and use the derivatives

$$\frac{dR(\zeta)}{d\zeta} = \frac{ds}{d\zeta} \times \frac{dR(\zeta)}{ds}, \quad \frac{d^2R(\zeta)}{d\zeta^2} = (2\zeta)^2 \frac{d^2R(\zeta)}{ds^2} + 2\frac{dR(\zeta)}{ds}. \quad (17)$$

Substituting Eq. (17) into Eq. (16), with the coordinate transformation $R(\zeta) \rightarrow \psi(s)$ we obtained

$$\psi''(s) + \frac{1}{2s}\psi'(s) + (\frac{-\frac{2\rho^2}{\hbar}s^2 + 2\epsilon s - l(l+1)}{4s^2})\psi(s) = 0. \quad (18)$$

Now comparing Eq. (18) with Eq. (6), we found

$$\gamma_1 = \frac{2\rho^2}{\hbar}, \gamma_2 = 2\epsilon \quad \gamma_3 = l(l+1), \quad (19)$$

and the parametric constants given in Eq. (9) are obtained as follows

$$\lambda_1 = 1, \quad \lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = 0, \ \lambda_6 = \gamma_1, \ \lambda_7 = -\gamma_2, \ \lambda_8 = l(l+1),$$
$$\lambda_9 = \gamma_1, \ \lambda_{10} = 1 + 2\sqrt{l(l+1)}, \quad \lambda_{11} = 2\sqrt{\gamma_1}, \quad \lambda_{12} = \sqrt{l(l+1)},$$
$$\lambda_{13} = -\sqrt{\gamma_1}. \quad (20)$$

Finally, substituting the appropriate terms in Eqs. (14), (19) and (20) into Eq. (7), we obtained the energy spectrum of the Gaussian well as

$$E_{nl} = \sqrt{\frac{2\hbar^2 V_0 \alpha}{m}} \left\{\left(n + \frac{1}{2}\right) + \sqrt{l(l+1)}\right\} - V_0, \quad (21)$$

and the wave function for the Gaussian well is obtained using Eq. (12) as

$$\psi_{nl}(s) = s^{\lambda_{12}} e^{\lambda_{13}s} L_n^{\lambda_{10}-1}(\lambda_{11}s) = N_n s^{\sqrt{l(l+1)}} e^{-\sqrt{\frac{2\rho^2}{\hbar}}s} L_n^{2\sqrt{l(l+1)}}\left(2\sqrt{\frac{2\rho^2}{\hbar}}\ s\right), \quad (22)$$

were $L_n^{2\sqrt{l(l+1)}}\left(2\sqrt{\frac{2\rho^2}{\hbar}}\ s\right)$ is the associated Laguerre polynomial.

RESULTS AND DISCUSSION

The eigenvalues in Eq. (21) for the ground state and first excited states are computed for s-wave ($l = 0$). We used the units $\hbar = 2m = 1$ and set $\alpha = 0.4$ for different potential well depth (V_0) as shown in table 1. The results for the ground state eigenvalues are in good agreement with the variational method for bound states solutions reported in Refs. 9 and 10. We note that the first excited energy values computed with our method are fairly in good agreement for the well depth of $V_0 \geq 10$ (see Fig. 1) as compared with the results in Ref. 9. While for potential barrier depth with $V_0 \leq 3$ would result in positive energies. This might be an indication that tunneling effect

ISSN 2055-009X(Print), ISSN 2055-0103(Online)

occurs for positive eigenvalues. The results of Chalk [17] for the transmission probability with the truncated Gaussian potential also show that tunneling effects occurs for all positive eigenvalues. However, when the screening parameter is set equal to zero ($\alpha = 0$), the particle is confined to the Gaussian well with the negative energy of $-V_0$.

Table 1. Approximate eigenvalues for the ground state E_{00} and first excited state E_{10}

V_0	NU method (present work) $(\mathbf{E_{00}})$	Variational method[9] $(\mathbf{E_{00}})$	Numerical solution[9] $(\mathbf{E_{00}})$	Variational Method[10] $(\mathbf{E_{00}})$	NU method (present work) $(\mathbf{E_{10}})$	Variational Method[9] $(\mathbf{E_{10}})$	Numerical method[9] $(\mathbf{E_{10}})$
1	-0.3675	-0.467	-0.47740	-0.4671			
2	-1.1056	-1.179	-1.18772			-0.01	-0.07543
2.5	-1.5000			-1.8005			
3	-1.9046	-1.956	-1.96372	-1.9557		-0.31	-0.36980
4	-2.7351	-2.767	-2.77449		-0.2053	-0.73	-0.78392
5	-3.5858	-3.601	-3.60765		-0.7574	-1.23	-1.27170
10	-8.0000	-7.948	-7.95267		-4.0000	-4.25	-4.28060
15	-12.5505	-12.446	-12.4500		-7.6515	-7.74	-7.76229
20	-17.1716	-17.023	-17.02623		-11.5147	-11.46	-11.48523
25	-21.8377	-21.650	-21.65289		-15.5132	-15.34	-15.36143
30	-26.5359	-26.312	-26.31538		-19.6077	-19.33	-19.34617

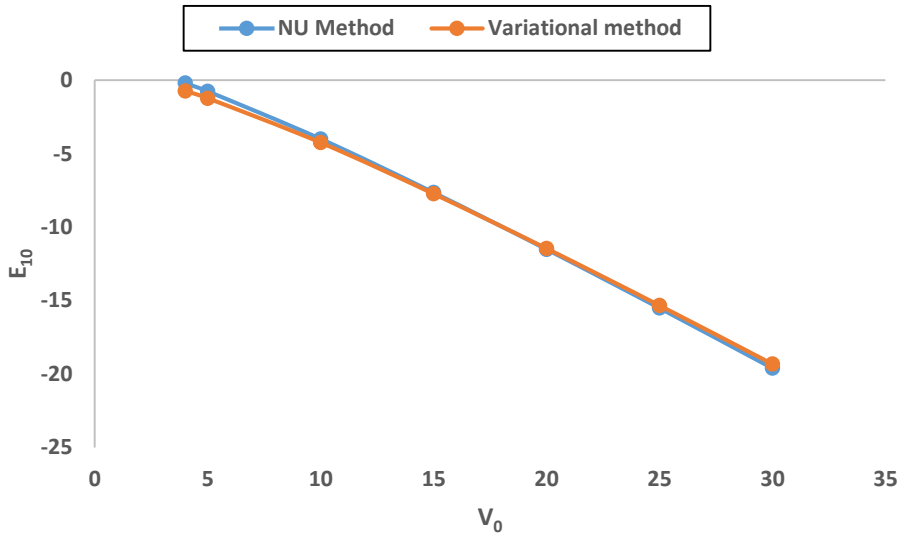

Figure 1: The energy of the first excited state as a function of the well depth V_0. The results obtained with the NU method are plotted with the results obtained using the variation method in Ref. 9

ISSN 2055-009X(Print), ISSN 2055-0103(Online)

CONCLUSION

We have obtained the bound-state solutions to the radial SE for a QMGP and the corresponding wave-function in closed form within the framework of the NU method. The approximate ground-state and first excited eigenvalues obtained for the s-wave are in good agreement with the variational method and numerical solution for sufficiently large potential depth. Equations (21) and (22) might be useful in analyzing the tunneling effects of a single particle confined in a QMGP well and in the studying of asymptotic behavior of other physical systems.

References

[1] P. C. W. Davies, and D. S. Betts, *Quantum Mechanics*, 2nd ed. (Chapman and Hall, London, 1994).

[2] M. Hamzavi, M. Movahedi, K. E. Thylve, and A. A. Rajabi, "Approximate Analytical Solution of the Yukawa Potential with Arbitrary Angular Momenta", Chin. Phys. Lett. **29**(8), 1-4 (2012).

[3] B. I. Ita *et al*., "Approximate Solution to the Schrodinger Equation with Manning-Rosen Plus a Class of Yukawa Potential via the WKBJ Approximation method". Bulg. J. Phys. **45**, 323-333 (2018).

[4] A. N. Ikot and L. E. Akpabio, "Approximate solution of the Schrodinger equation with Rosen-Morse potential including the centrifugal term", Appl. Phys. Res. **2**(2), 202-208 (2010).

[5] B.I. Ita *et al*. "Radial solution of the s-wave D-dimensional non-relativistic Schrodinger equation for generalized Manning-Rosen and Mie type nuclei potential within the framework of parametric Nikiforov-Uvarov method", Journal of Nigerian Association of Mathematical Physics. **36**(2), 193-198 (2016).

[6] B.I. Ita, *et al*. "Approximate solution of the N-dimensional radial Schrodinger equation with Kratzer plus reduced pseudo-harmonic oscillator potential within the framework of parametric Nikiforov-Uvarov method", Journal of Nigerian Association of Mathematical Physics. **36**(2), 199-204 (2016).

[7] H. Louis *et al*. "WKB solution for quantum mechanical gravitational potential plus harmonic oscillator potential", International Research Journal of pure and Applied Physics. **5**(3) 27-32. (2017).

[8] E. Omugbe, "Determination of energy levels of a quantum bouncing ball with the numerical support of Maple computer program", Physical science international journal **20**(3), 1-5 (2018).

[9] F. M. Fernandez, "Quantum Gaussian wells and barriers", Am. J. Phys. **79**(7) 752-754 (2011).

[10] S. Nandi, "The quantum Gaussian well", Am. J. Phys. **78** 1341-1345 (2010). e-print arXiv: 10113637v1

ISSN 2055-009X(Print), ISSN 2055-0103(Online)

[11] H. Mutuk, "Asymptotic iteration and variational methods for Gaussian potential", Pramana J. Phys. **92**(66), 1-5 (2019).

[12] F. M. Fernandez, Q. Ma, and R. H. Tipping, "Tight upper and lower bounds for energy eigenvalues of the Schrodinger equation", Phys Rev. A. **39,** 1606-1609 (1989).

[13] F. M. Fernandez, "Wronskian method for bound states", Eur. J. Phys. **32**, 723-732 (2011).

[14] A. Chatterjee, "$1/N$ Expansion for the Gaussian potential", J. Phys. A**. 18**(12), 2403-2408 (1985).

[15] A. F. Nikiforov and V. B. Uvarov, Special functions of mathematical physics (Birkhauser, Basel, 1988).

[16] C. Tezcan and, R. Sever, "A general approach for the exact solution of the Schrödinger equation", International journal of theoretical physics. **48**, 337-350 (2009).

[17] J.D. Chalk, "A study of barrier penetration in quantum mechanics", Am.J. Phys**. 56**, 29-32 (1988).

ISSN 2055-009X(Print), ISSN 2055-0103(Online)