Polynomial Solutions of Shcrödinger Equation with the Generalized Woods–Saxon Potential

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Abstract

The bound state energy eigenvalues and the corresponding eigenfunctions of the generalized Woods-Saxon potential are obtained in terms of the Jacobi polynomials. Nikiforov-Uvarov method is used in the calculations. It is shown that the results are in a good agreement with the ones obtained before.

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1 Introduction

Exact solution of Schrödinger equation for central potentials has generated much interes in recent years. So far, these potentials are the parabolic type potential [1], the Eckart potential [1, 2, 3], the Fermi-step potential [2, 3], the Rosen- Morse potential [4], the Ginocchio barrier [5], the Scarf barrier [6], the Morse potential [7] and a potential which interpolates between Morse and Eckart barriers [8]. In addition, many authors have studied on exponential type potentials [9, 10, 11, 12, 13] and quasi exactly solvable quadratic potentials [14, 15, 16]. The exact solutions for these models have been obtained analytically.

Recently, an alternative method known as the Nikiforov-Uvarov (NU) method has been introduced for solving the Schrödinger equation (SE). There have been several applications of SE with some well-known potentials [17, 18, 19], Dirac, Klein-Gordon and Duffin-Kemmer-Petiau equations for a Coulomb type potential by using this method as well [21, 22, 23].

In the present work, the real-valued bound-state energies of the generalized Woods-Saxon potential are evaluated through the NU Method [24] by following the framework of quantum mechanics. This method is based on solving the time-independent Schrödinger equation by reduction to a generalized equation of hypergeometric type. Energy eigenvalues and the corresponding eigenfuctions are calculated exactly. The generalized Wood-Saxon potential as a shell model is selected. It can be used for describing metallic clusters in a successful way and for lighting the central part of the interaction neutron with one heavy nucleus [25, 26].

This paper is arranged as follows: In Sec. II we introduce the NU method. In Sec. III we apply the method to solve the Schrödinger equation with the generalized Woods-Saxon potential. Shapes of the potential and energy are studied in Sec. IV. In Sec. V we discuss the results.

2 Nikiforov-Uvarov Method

The NU method provides us an exact solution of non-relativistic Schrödinger equation for certain kind of potentials [24]. The method is based on the solutions of general second order linear differential equation with special orthogonal functions [27]. For a given real or complex potential, the Schrödinger equation in one dimension is reduced to a generalized equation of

hypergeometric type with an appropriate s = s(x) coordinate transformation. Thus it can be written in the following form,

$$\psi''(s) + \frac{\widetilde{\tau}(s)}{\sigma}\psi'(s) + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0$$
(1)

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most second-degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. To find a particular solution of Eq.(1) by separation of variables, we use the following the transformation

$$\psi(s) = \phi(s)y(s) \tag{2}$$

This reduces Schrödinger equation, Eq.(1), to an equation of hypergeometric type,

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0, \tag{3}$$

where $\phi(s)$ satisfies $\phi(s)'/\phi(s) = \pi(s)/\sigma(s)$. y(s) is the hypergeometric type function whose polynomial solutions are given by Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} \left[\sigma^n(s) \rho(s) \right],\tag{4}$$

where B_n is a normalizing constant and the weight function ρ must satisfy the condition [24]

$$(\sigma\rho)' = \tau\rho. \tag{5}$$

The function π and the parameter λ required for this method are defined as

$$\pi = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma} \tag{6}$$

and

$$\lambda = k + \pi'. \tag{7}$$

Here, $\pi(s)$ is a polynomial with the parameter s and the determination of k is the essential point in the calculation of $\pi(s)$. Thus, in order to find the value of k, the expression under the square root must be square of a polynomial. Hence, a new eigenvalue equation for the Schrödinger equation becomes

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', \quad (n = 0, 1, 2, ...)$$
(8)

where

$$\tau(s) = \widetilde{\tau}(s) + 2\pi(s), \tag{9}$$

and it will have a negative derivative.

3 Generalized Woods–Saxon Potential

The interactions between nuclei are commonly described by using a potential that consist of the Coulomb and the nuclear potentials. These potentials are usually taken to be of the Woods-Saxon form. As an example it can be given as the generalized Woods-Saxon potential [28] $(r=R_{0})$

$$V(r) = -\frac{V_0}{1 + e^{\left(\frac{r-R_0}{a}\right)}} - \frac{C.e^{\left(\frac{r-R_0}{a}\right)}}{\left(1 + e^{\left(\frac{r-R_0}{a}\right)}\right)^2} , \qquad (10)$$

where V_0 is the potential depth, R_0 is the width of the potential and a is the surface thickness which is usually adjusted to the experimental values of ionization energies. In order to calculate the energy eigenvalues and the corresponding eigenfunctions, the potential function given by Eq.(10) is substituted into the radial part of Schrödinger equation:

$$\psi''(r) + \frac{2m}{\hbar^2} \left[E + \frac{V_0}{1 + qe^{2\alpha r}} + \frac{Ce^{2\alpha r}}{\left(1 + qe^{2\alpha r}\right)^2} \right] \psi(r) = 0.$$
(11)

Here, some assignments are made in the radial Schrödinger equation such as $R(r) = \psi(r)/r$, $r - R_0 \equiv r$ and $1/a \equiv 2\alpha$. In addition, q is deformation parameter and an arbitrary real constant within the potential.

Now, in order to apply the NU–method, we rewrite Eq.(11) by using a new variable of the form $s = -e^{2\alpha r}$,

$$\frac{d^2\psi(s)}{ds^2} + \frac{1}{s}\frac{d\psi(s)}{ds} + \frac{m}{2\hbar^2\alpha^2 s^2} \left[E + \frac{V_0}{(1-qs)} - \frac{Cs}{(1-qs)^2}\right]\psi(s) = 0.$$
 (12)

By introducing the following dimensional parameters

$$\varepsilon = -\frac{mE}{2\hbar^2 \alpha^2} > 0 \quad (E < 0), \qquad \beta = \frac{mV_0}{2\hbar^2 \alpha^2} \quad (\beta > 0), \qquad \gamma = \frac{mC}{2\hbar^2 \alpha^2} \quad (\gamma > 0) \tag{13}$$

which leads to a hypergeometric type equation defined in Eq.(1):

$$\frac{d^2\psi(s)}{ds^2} + \frac{1-qs}{s(1-qs)}\frac{d\psi(s)}{ds} + \frac{1}{s^2(1-qs)^2} \times \left[-\varepsilon q^2 s^2 + (2\varepsilon q - \beta q - \gamma)s + \beta - \varepsilon\right]\psi(s) = 0.$$
(14)

After the comparison of Eq.(14) with Eq.(1), we obtain the corresponding polynomials as

$$\widetilde{\tau}(s) = 1 - qs, \quad \sigma(s) = s(1 - qs), \quad \widetilde{\sigma}(s) = -\varepsilon q^2 s^2 + (2\varepsilon q - \beta q - \gamma)s + \beta - \varepsilon.$$
 (15)

Substituting these polynomials into Eq.(6), we obtain π function as

$$\pi(s) = -\frac{qs}{2} \pm \frac{1}{2}\sqrt{\left(q^2 + 4\varepsilon q^2 - 4kq\right)s^2 + 4\left(\beta q + \gamma - 2\varepsilon q + k\right)s + 4\left(\varepsilon - \beta\right)}$$
(16)

taking $\sigma'(s) = 1 - 2qs$. The discriminant of the upper expression under the square root has to be zero. Hence, the expression becomes the square of a polynomial of first degree;

$$\left(q^2 + 4\varepsilon q^2 - 4kq\right)s^2 + 4\left(\beta q + \gamma - 2\varepsilon q + k\right)s + 4\left(\varepsilon - \beta\right) = 0,$$
(17)

and

$$\Delta = \left[4\left(\beta q + \gamma - 2\varepsilon q + k\right)\right]^2 - 4 \times 4\left(\varepsilon - \beta\right)\left(q^2 + 4\varepsilon q^2 - 4kq\right) = 0.$$
(18)

When the required arrangements are done with respect to the constant k, its double roots are derived as $k_{1,2} = (\beta q - \gamma) \pm q \sqrt{(\varepsilon - \beta) (1 + \frac{4\gamma}{q})}$.

Thus substituting, these values for each k into Eq.(16) following possible solution is obtained for $\pi(s)$

$$\pi(s) = -\frac{qs}{2} \pm \frac{1}{2} \begin{cases} \left[(2\sqrt{\varepsilon - \beta} - \sqrt{1 + \frac{4\gamma}{q}})qs - 2\sqrt{\varepsilon - \beta} \right], & \text{for} \quad k = (\beta q - \gamma) + q\sqrt{(\varepsilon - \beta)(1 + \frac{4\gamma}{q})} \\ \left[(2\sqrt{\varepsilon - \beta} + \sqrt{1 + \frac{4\gamma}{q}})qs - 2\sqrt{\varepsilon - \beta} \right], & \text{for} \quad k = (\beta q - \gamma) - q\sqrt{(\varepsilon - \beta)(1 + \frac{4\gamma}{q})} \\ (19) \end{cases}$$

It is clearly seen that the energy eigenvalues are found with a comparison of Eq.(7) and Eq.(8). From the four possible forms of the polynomial $\pi(s)$ we select the one for which the function $\tau(s)$ in Eq.(9) has a negative derivative. Therefore, the function $\tau(s)$ satisfies these requirements, with

$$\tau(s) = 1 - 2qs - \left(\left(2\sqrt{\varepsilon - \beta} + \sqrt{1 + 4\gamma/q} \right) qs - 2\sqrt{\varepsilon - \beta} \right),$$

$$\tau'(s) = -2q - \left(2\sqrt{\varepsilon - \beta} + \sqrt{1 + 4\gamma/q} \right) q.$$
(20)

Hence, the polynomial $\pi(s)$ is computed from Eq.(16) as

$$\pi(s) = -\frac{qs}{2} - \frac{1}{2} \left[\left(2\sqrt{\varepsilon - \beta} + \sqrt{1 + 4\gamma/q} \right) qs - 2\sqrt{\varepsilon - \beta} \right].$$
(21)

From Eq.(8) we also get

$$\lambda = (\beta q - \gamma) - q\sqrt{(\varepsilon - \beta)(1 + 4\gamma/q)} - \frac{q}{2} - \frac{1}{2} \left[(2\sqrt{\varepsilon - \beta} + \sqrt{1 + 4\gamma/q}) q \right],$$
(22)

and also

$$\lambda = \lambda_n = nq \left(2(1 + \sqrt{\varepsilon - \beta}) + \sqrt{1 + 4\gamma/q} \right) + n(n-1)q.$$
(23)

It is seen that the parameter ε has the following form

$$\varepsilon_{nq} = \frac{1}{16} \left[\sqrt{1 + \frac{4\gamma}{q}} + (1 + 2n) \right]^2 + \frac{\beta^2}{\left[\sqrt{1 + \frac{4\gamma}{q}} + (1 + 2n) \right]^2} + \frac{\beta}{2}$$
(24)

Substituting the values of ε and β into Eq.(13) and by using the transformation $2\alpha \equiv 1/a$ in Eq.(22), one can immediately determine the energy eigenvalues E_{nq} as

$$E_{nq} = -\frac{\hbar^2}{2ma^2} \left\{ \frac{1}{16} \left[\sqrt{1 + \frac{8mCa^2}{\hbar^2 q}} + (1+2n) \right]^2 + \frac{4\left(\frac{mV_0a^2}{\hbar^2}\right)^2}{\left[\sqrt{1 + \frac{8mCa^2}{\hbar^2 q}} + (1+2n) \right]^2} + \frac{mV_0a^2}{\hbar^2} \right\}.$$
(25)

Here, the index n is non-negative integers with $\infty > n \ge 0$ and the above equation indicates that we deal with a family of the generalized Woods-Saxon potential. Of course it is clear that by imposing appropriate changes in the parameters a and V_0 , the index n describes the quantization for the bound states and the energy spectrum. In addition, if the parameter C in Eq.(25) is adjusted to zero, solution reduces to the form obtained for the standard Woods-Saxon potential without regarding the parameter q.

Let us now find the corresponding wave eigenfunctions. Due to the NU-method, the polynomial solutions of the hypergeometric function y(s) depend on the determination of weight function $\rho(s)$ which is satisfies the differential equation $[\sigma(s)\rho(s)]' = \tau(s)\rho(s)$. Thus, $\rho(s)$ is calculated as

$$\rho(s) = (1 - qs)^{\nu - 1} s^{2\sqrt{\varepsilon - \beta}},$$
(26)

where $\nu = 1 + \sqrt{1 + \frac{4\gamma}{q}}$. Substituting into the Rodrigues relation given in Eq.(4), the eigenfunctions are obtained in the following form

$$y_{nq}(s) = B_n \left(1 - qs\right)^{-(\nu-1)} s^{-2\sqrt{\varepsilon-\beta}} \frac{d^n}{ds^n} \left[\left(1 - qs\right)^{n+\nu-1} s^{n+2\sqrt{\varepsilon-\beta}} \right],$$
(27)

where B_n is the normalization constant and its value is 1/n!. Choosing q = 1, the polynomial solutions of $y_n(s)$ are expressed in terms of Jacobi Polynomials, which is one of the orthogonal polynomials with weight function $(1 - s)^{\nu-1}s^{2\sqrt{\varepsilon-\beta}}$ in the closed interval [0, 1], giving [constant] $P_n^{(2\sqrt{\varepsilon-\beta}, \nu-1)}(1-2s)$ [27]. By substituting $\pi(s)$ and $\sigma(s)$ into the expression

 $\phi(s)'/\phi(s) = \pi(s)/\sigma(s)$ and solving the resulting differential equation, the other part of the wave function in Eq.(2) is found as

$$\phi(s) = (1-s)^{\mu} s^{\sqrt{\varepsilon-\beta}}, \qquad (28)$$

where $\mu = \nu/2$ and again taking q = 1. Combining the Jacobi polynomials and $\phi(s)$ in Eq.(28), the s-wave functions are constructed as

$$\psi_n(s) = A_n s^{\sqrt{\varepsilon - \beta}} (1 - s)^{\mu - \nu + 1} P_n^{(2\sqrt{\varepsilon - \beta}, \nu - 1)} (1 - 2s),$$
(29)

where A_n is a new normalization constant.

4 Potential and Energy Eigenvalue Shapes

For the generalized Woods-Saxon potential in Eq.(10), the potential shape can be determined by the parameters V_0 , a and C. Therefore, we have adopted a generalized Woods-Saxon shape for the real part of the optical-model potential [29] and investigated the scattering phenomenon for this potential only. The empirical values found by Perey et al. [30] $r_0 = 1.285 \ fm$, $a = 0.65 \ fm$ and $V_0 \approx 40.5 + 13A \ MeV$ are used. Here, A is the mass number of target nucleus and $R_0 = r_0 A^{1/3}$. The shape of the generalized Woods-Saxon potential given by Eq.(10) is illustrated in Fig.1.

Fig.2 shows that the energy eigenvalues as a function of the discrete level n for different values of the parameter a. Of course it is clear that by imposing appropriate changes in the parameters a and V_0 , the index n describes the quantization of the bound states and the energy spectrum. Some of the initial energy levels for q = 1 value are presented by choosing $C = 10 \ MeV$, A = 56 which is the geometric average of the target mass number $44 \le A \le 72$ [31].

5 Conclusions

The exact solutions of the radial Schrödinger equation for the generalized Woods-Saxon potential with the zero angular momentum are obtained. Eigenvalues and eigenfunctions obtained from the real form of the potential are computed. So, the wave functions are physical and energy eigenvalues are in a good agreement with the results obtained by the other methods. Nikiforov-Uvarov method is used in the calculations. We have seen that there were some restriction on the potential parameters for the bound states within the framework of quantum mechanics. That is, the value of C from the potential parameters is increased for the constant value of the parameter a, it is seen that the depth of potential increases rapidly. Therefore, if all the parameters of potential remain purely real, it is clear that all bound energies E_n with $n \ge 0$ represent a negative energy spectrum. We also point out that the exact results obtained for the generalized Woods-Saxon potential may have some interesting applications in the study of different quantum mechanical and the nuclear scattering systems.

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Figure Captions

Figure 1: Variation of the generalized Woods-Saxon potential as a function of r.

Figure 2: The variation of the energy eigenvalues with respect to the quantum number n with $V_0 \approx 48$ MeV. The curves correspond to the different values of the range parameter a.



