Polynomial solutions of the Schrödinger equation for the generalized Woods-Saxon potential

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(Received 6 December 2004; published 17 August 2005)

The bound state energy eigenvalues and the corresponding eigenfunctions of the generalized Woods-Saxon potential are obtained by means of Nikiforov-Uvarov (NU) method. Certain bound states of the Schrödinger equation for the potential are calculated analytically and the wave functions are found in terms of the Jacobi polynomials. It is shown that the results are in good agreement with those obtained previously.

DOI: 10.1103/PhysRevC.72.027001 PACS number(s): 21.60.Cs, 03.65.Ge, 02.30.Gp, 24.10.Ht

Exact solution of the Schrödinger equation for the central potentials has generated much interest in recent years. So far, these potentials are the parabolic type potential [1], the Eckart potential [1–3], 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 exponential type potentials [9–13] and quasi-exact-solvable quadratic potentials [14–16]. 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 involving the SE with some well-known potentials [17,18], and the Dirac, Klein-Gordon, and Duffin-Kemmer-Petiau equations for the exponential type potentials using this method as well [19–22]. It is well known that the Woods-Saxon potential is one of the exponential type potentials. This potential plays an essential role in nuclear physics since it can be used to describe the interaction of a neutron with a heavy nucleus. Thus, one can need to obtain the energy eigenvalues and corresponding eigenfunctions of the one particle within the potential. In this case, the exact bound states of Woods-Saxon potential in the presence of an additional potential term can be calculated by means of NU method. This extra term added to the Woods-Saxon potential is named "generalized" and hence it is appeared as the generalized Woods-Saxon potential.

In the present work, the bound-state solutions of the generalized Woods-Saxon potential are evaluated using the NU Method [23] by following the framework of quantum mechanics. This method is based on solving the time-independent Schrödinger equation by reduced to a generalized equation of the hypergeometric type. After that, energy eigenvalues and the corresponding eigenfunctions are exactly calculated by NU method for s waves only. In addition, this method can be used for describing metallic clusters successfully and for lighting the central part of the neutron interaction with a heavy nucleus [24,25].

The NU method provides an exact solution of the nonrelativistic Schrödinger equation for certain kinds of potentials [23]. The method is based on the solution of general second order linear differential equations with special orthogonal functions [26]. In the framework of this method, the one-dimensional Schrödinger equation is reduced to a generalized equation of the hypergeometric type with an appropriate $s = s(x)$ coordinate transformation. Thus it can be written in the following form:

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

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 transformation:

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

This selection reduces the Schrödinger equation, Eq. (1), to an equation of the 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

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

where B_n is the normalization constant and the weight function ρ must satisfy the condition [23]

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

The function π and the parameter λ 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 depended on the function $s(x)$. On the other hand, in order to find the value of k, the expression under the square root must be square of a polynomial.

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This is possible only if its discriminant is zero. Hence, a new eigenvalue equation for the Schrödinger equation becomes

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

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \quad (9)$$

and it will have a negative derivative.

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. Here, we consider the generalized Woods-Saxon potential [27]

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

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. We begin by looking for solutions that are separable into products; $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$ and putting this into the time-independent Schrödinger equation. Afterward, we calculate the energy eigenvalues and the corresponding eigenfunctions by using the following radial part of Schrödinger equation:

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

Here, we take $R(r) = \psi(r)/r$, $r - R_0 \equiv r$, and $1/a \equiv 2\alpha$. In addition, q is a real parameter.

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

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

We introduce the following dimensional parameters:

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

$$\gamma = \frac{mC}{2\hbar^2\alpha^2} \quad (\gamma > 0),$$

which leads to a hypergeometric-type equation

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

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

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

Substituting these polynomials into Eq. (6) and by taking $\sigma'(s) = 1 - -2qs$, we obtain $\pi(s)$ polynomial as

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

According to the NU method, the expression in the square root must be the square of a polynomial. So, one can find possible functions for each k as follows:

$$\pi(s) = -\frac{qs}{2} \pm \frac{1}{2}\begin{cases} \left[\left(2\sqrt{\varepsilon - \beta} - \sqrt{1 + \frac{4\gamma}{q}}\right)qs - 2\sqrt{\varepsilon - \beta}\right], & \text{for} \quad k = (\beta q - \gamma) + q\sqrt{(\varepsilon - \beta)\left(1 + \frac{4\gamma}{q}\right)} \\ \left[\left(2\sqrt{\varepsilon - \beta} + \sqrt{1 + \frac{4\gamma}{q}}\right)qs - 2\sqrt{\varepsilon - \beta}\right], & \text{for} \quad k = (\beta q - \gamma) - q\sqrt{(\varepsilon - \beta)\left(1 + \frac{4\gamma}{q}\right)}. \end{cases} \quad (17)$$

It is clearly seen that the energy eigenvalues are found by comparing Eqs. (7) and (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 $\tau(s)$ satisfying this requirement is determined

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

and its derivative is obtained

$$\tau'(s) = -2q - (2\sqrt{\varepsilon - \beta} + \sqrt{1 + 4\gamma/q})q. \quad (18)$$

Hence, the polynomial $\pi(s)$ is computed from Eq. (17) as

$$\pi(s) = -\frac{qs}{2} - \frac{1}{2}[(2\sqrt{\varepsilon - \beta} + \sqrt{1 + 4\gamma/q})qs - 2\sqrt{\varepsilon - \beta}]. \quad (19)$$

From Eq. (8) we achieve

$$\lambda = (\beta q - \gamma) - q\sqrt{(\varepsilon - \beta)(1 + 4\gamma/q)} - \frac{q}{2} - \frac{1}{2}[(2\sqrt{\varepsilon - \beta} + \sqrt{1 + 4\gamma/q})q], \quad (20)$$

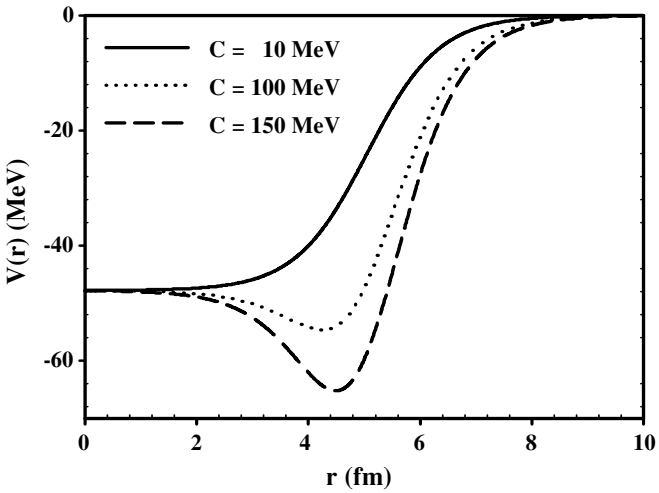

FIG. 1. Variation of the generalized Woods-Saxon potential as a function of r.

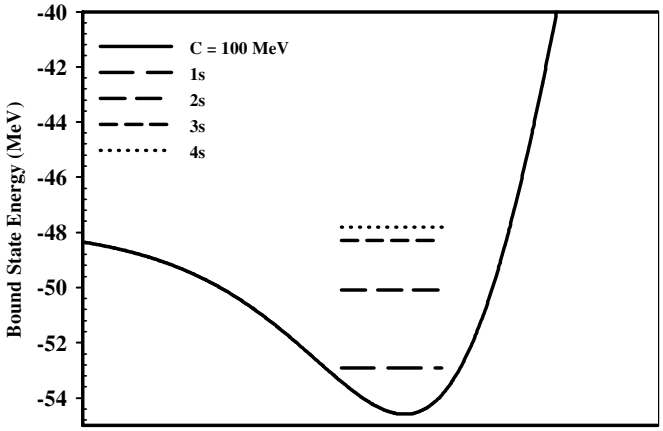

FIG. 2. The bound state energy spectrum for each excitation energy. The horizontal lines denote the variation of the energy eigenvalues with respect to the principle quantum number for $C = 100$ MeV.

and also

$$\lambda = \lambda_n = nq[2(1+\sqrt{\varepsilon-\beta}) + \sqrt{1+4\gamma/q}] + n(n-1)q, \qquad (n = 0, 1, 2, \ldots). \quad (21)$$

It is seen that the parameter ε has the following form:

$$\varepsilon_{nq} = \frac{1}{16}\left[\sqrt{1+\frac{4\gamma}{q}} + (1+2n)\right]^2 + \frac{\beta^2}{\left[\sqrt{1+\frac{4\gamma}{q}} + (1+2n)\right]^2} + \frac{\beta}{2}. \quad (22)$$

Substituting the values of ε and β into Eq. (13) and by using the transformation $2\alpha \equiv 1/a$ in Eq. (20), one can immediately determine the energy eigenvalues E_{nq} as

$$E_{nq} = -\frac{\hbar^2}{2ma^2}\left\{\frac{1}{16}\left[\sqrt{1+\frac{8mCa^2}{\hbar^2 q}} + (1+2n)\right]^2 + \frac{4\left(\frac{mV_0a^2}{\hbar^2}\right)^2}{\left[\sqrt{1+\frac{8mCa^2}{\hbar^2 q}} + (1+2n)\right]^2} + \frac{mV_0a^2}{\hbar^2}\right\}. \quad (23)$$

where n stands for the radial quantum number [28]. If the parameter C in Eq. (23) is adjusted to zero, the solution is reduced to the form obtained for the standard Woods-Saxon potential for the case of $q = 1$.

Let us now find the corresponding eigenfunctions. The polynomial solutions of the hypergeometric function $y(s)$ depend on the determination of weight function $\rho(s)$ satisfying the differential equation $[\sigma(s)\rho(s)]' = \tau(s)\rho(s)$. Thus, $\rho(s)$ is calculated as

$$\rho(s) = (1-qs)^{\nu-1}\, s^{2\sqrt{\varepsilon-\beta}}, \quad (24)$$

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:

$$y_{nq}(s) = B_n\,(1-qs)^{-(\nu-1)}\, s^{-2\sqrt{\varepsilon-\beta}}\frac{d^n}{ds^n} \times [(1-qs)^{n+\nu-1} s^{n+2\sqrt{\varepsilon-\beta}}], \quad (25)$$

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]$P_n^{(2\sqrt{\varepsilon-\beta},\nu-1)}(1-2s)$. 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

$$\phi(s) = (1-s)^{\mu} s^{\sqrt{\varepsilon-\beta}}, \quad (26)$$

where $\mu = \nu/2$ and again $q = 1$. Combining the Jacobi polynomials and $\phi(s)$ in Eq. (26), the s-wave functions are constructed as

$$\psi_n(s) = A_n s^{\sqrt{\varepsilon-\beta}}(1-s)^{\mu-\nu+1} P_n^{(2\sqrt{\varepsilon-\beta},\nu-1)}(1-2s), \quad (27)$$

where A_n is a new normalization constant.

We have adopted a generalized Woods-Saxon shape for the real part of the optical-model potential [29] and investigated the scattering phenomenon. The empirical values found by Perey *et al.* are given as $r_0 = 1.285$ fm and $a = 0.65$ fm [30]. In addition, the following Woods-Saxon parameter is calculated by $V_0 \approx 40.5 + 0.13A$ MeV. Here, A is the atomic mass number of target nucleus and $R_0 = r_0 A^{1/3}$. The variation of the generalized Woods-Saxon potential given by Eq. (10) is illustrated in Fig. 1. It is clearly seen from Fig. 1 that the potential depth increases when the parameter C is increased from 10 to 150 MeV. In this way, one can say that whether the bound states exist within the potential.

The bound state energies for each excitation energy are given with horizontal lines sketched to the potential for $C = 100$ and $C = 150$ MeV in Figs. 2 and 3, respectively.

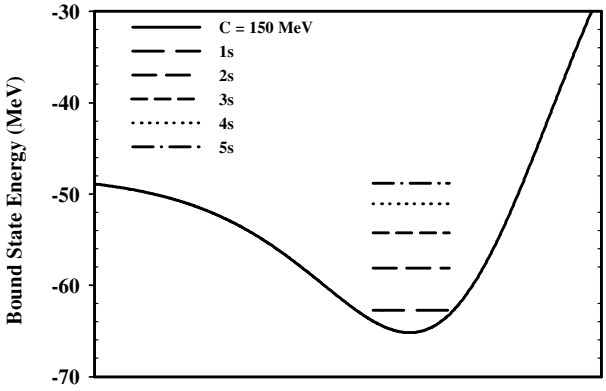

FIG. 3. The bound state energy spectrum for each excitation energy. The horizontal lines denote the variation of the energy eigenvalues with respect to the principle quantum number for $C = 150$ MeV.

Some of the initial energy levels for $q = 1$ are presented by choosing $A = 56$, which is the geometric average of the target atomic mass number $44 \leqslant A \leqslant 72$ [31]. It is emphasized that there is no bound state in the potential when the parameter C is equal to 10 MeV.

The exact solutions of the radial Schrödinger equation for the generalized Woods-Saxon potential with the zero angular momentum are obtained by using NU method. Eigenvalues and eigenfunctions obtained from the real form of the potential are computed analytically. It is seen that the Nikiforov-Uvarov method used in the calculations is more suitable and systematical method to solve the Schrödinger equation. In addition, we have seen that there are some restrictions on the potential parameters for the bound state solutions within the framework of quantum mechanics. That is, when the value of the parameter C is increased for the constant value of the parameter a, it is determined that the depth of potential increases rapidly. In this case, we obtained the bound state energies. Therefore, if all the parameters of potential remain purely real, it is clear that all bound state energies E_n represent a negative energy spectrum under the conditions of $3 \geqslant n \geqslant 0$ for $C = 100$ and $5 \geqslant n \geqslant 0$ for $C = 150$ MeV. 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. Consequently, the wave functions are physical and energy eigenvalues are in good agreement with the results obtained by the other methods.

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