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Solutions of Woods–Saxon Potential with Spin-Orbit and Centrifugal Terms through Nikiforov–Uvarov Method

M.R. Pahlavani* and S.A. Alavi†

Department of Nuclear Physics, Faculty of Sciences, Mazandaran University, P.O. Box 47415-416, Babolsar, Iran

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Abstract *In this study, the analytical solutions of the radial Schrödinger equation for the central Woods–Saxon potential together with spin-orbit interaction and centrifugal terms have been derived by using Nikiforov-Uvarov method. The energy eigenvalues and corresponding eigenfunctions of nucleons have been obtained for various values of n, l, and j quantum numbers. The obtained results using this method are in satisfactory agreement with available data in the special case.*

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Key words: Schrödinger equation, spin-orbit interaction, Woods–Saxon potential, Nikiforov–Uvarov method

1 Introduction

The wave function as solutions of the Schrödinger differential equation, in non-relativistic quantum mechanics, and corresponding eigenenergy for a physical systems contain all possible information about the physical properties of a system. The exact solutions of the Schrödinger equation for different potentials have been derived and widely used in adverse fields of molecular, atomic, nuclear, and subnuclear physics. The exact analytic solutions of hydrogen atom and harmonic oscillator problem with complete set of potentials with any arbitrary l-state, as two fundamental examples in atomic and subatomic physics, have been represented in some literatures deliberately.[1–3] Up to now several methods have been used for solving the Schrödinger equation analytically. Such as the variational,[4–6] supersymmetry,[7–10] asymptotic iteration method,[9,11] the perturbation ladder operators method,[12] and Nikiforov–Uvarov Method (NU).[13–14]

The NU method has been successful to solve different second-order differential equations in both relativistic and non-relativistic quantum mechanics. Recently, this method has been used to find exact solution of the Schrödinger equation for several well known potentials, such as harmonic oscillator, Coulomb, Kratzer, Morse, Hulthen, Rosen–Morse, pseudoharmonic, Mie, Pöschl–Teller, and Woods–Saxon potentials[15–22] in non-relativistic quantum mechanics and for deriving analytic solution of the Dirac, Klein–Gordon, Salpeter and Duffin–Kemmer–Petiau (DKP) equations[17,23–25] in relativistic quantum mechanics.

The Woods–Saxon potential, as an important mean-field nuclear potential describes the interaction of single nucleon with whole nuclei and widely used in nuclear structure, nuclear reactions, nuclear scattering and particle physics, has been attracted a great deal of interest for some decades. In order to study the structure of nuclei contain, particle-hole theory, many nucleon configuration, electromagnetic transitions and nuclear decay the Woods–Saxon basis has been used as better choice than harmonic oscillator basis in both relativistic and non-relativistic theories of nuclear mean-field shell model.[4,26–30]

The single nucleon wave function, as fundamental parameter for studying nuclear structure and constructing the wave function of nuclei, is derived from single nucleon Schrödinger equation. The single-nucleon radial Schrödinger equation for a central potential can be written as

$$\Big[\frac{-\hbar^2}{2m}\Big(\nabla_r^2-\frac{l(l+1)}{r^2}\Big)+V(r)\Big]\psi(r)=E\psi(r)\,,\qquad(1)$$

where $V(r)$ is potential energy which is felt by single-nucleon and consists of the nuclear part for both neutron and proton and Coulomb part only for protons, and

$$V_{\rm c.f}=\frac{\hbar^2 l(l+1)}{2mr^2}$$

is known as centrifugal potential. By introducing the reduced radial wave function, $R(r)=r\psi(r)$, which is normalized by $\int|\psi(\vec{r})^r\,\mathrm{d}^3r=1$, Eq. (1) is rewritten as

$$\frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2}+\frac{2m}{\hbar^2}\Big[E-V(r)-\frac{\hbar^2 l(l+1)}{2mr^2}\Big]R(r)=0\,.\qquad(2)$$

The standard Woods–Saxon potential, as mean-field nuclear potential is given as,

$$V_{\rm WS}=\frac{-V_0}{1+\mathrm{e}^{(r-R_0)/a}}\,,\qquad(3)$$

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*E-mail: m.pahlavani@umz.ac.ir

†E-mail: a.alavi@stu.umz.ac.ir

where $V_0 = 40.5 + 0.13A$ MeV is the potential depth, $a = 0.65$ fm is surface diffuseness, $R_0 = r_0 A^{1/3}$ the radius of the spherical nucleus, $r_0 = 1.27$ fm, and A the mass number of nuclei. The Woods–Saxon potential alone does not reproduce experimentally observed magic numbers, which are indicated closed shelled nuclei. Including the spin-orbit interaction term to the mean field potential it is possible to reproduce these numbers. The spin-orbit term in mean-field shell model is defined as

$$V_{\rm LS}(r) = V_{\rm LS}^{(0)}\Big(\frac{r_0}{\hbar}\Big)^2 \frac{1}{r}\Big[\frac{\rm d}{{\rm d}r}\frac{1}{1+{\rm e}^{(r-R_0)/a}}\Big](\boldsymbol{L}\cdot\boldsymbol{S})\,, \tag{4}$$

where $V_{\rm LS}^{(0)} = 0.44V_0$. Therefore the complete form of the mean-field nuclear potential for single neutron is

$$V(r) = V_{\rm WS}(r) + V_{\rm LS}(r)\,. \tag{5}$$

Because of vast applications of Woods–Saxon basis for both spherical and deformed nuclei in nuclear and particle physics, the analytic solution of Woods–Saxon potential can be very useful and give valuable theoretical results. Recently by means of NU method the DKP equation is solved analytically for a vector deformed Woods–Saxon potential.[25] The exact solutions of S states ($l = 0$) and approximate analytic solutions of any l states for Woods–Saxon potential are available in literatures.[3,10,17–19,31]

Since the single-nucleon radial Schrödinger equation for this complicated potential Eq. (2) has not been solved for any j and l quantum numbers exactly, in this study, we attempt to solve this equation by using some approximations which transforms the Schrödinger equation into the form of NU differential equation that can be solved analytically. In Sec. 2, the formalism of NU method for solving specials types of differential equations is given. In Sec. 3, by introducing some new variables and using some approximation and expansions the solutions of radial Schrödinger equation for the complete set of potentials for neutron single particle are represented.

2 Formalism of Nikiforov–Uvarov Method

The NU method is constructed to solve the hypergeometric type second-order differential equations by means of the special orthogonal functions.[13] This method can be used to solve following second-order differential equations with an appropriate coordinate transformation $z = z(r)$,

$$\psi''(z) + \frac{\tilde\tau(z)}{\sigma(z)}\psi'(z) + \frac{\tilde\sigma(z)}{\sigma(z)^2}\psi(z) = 0\,, \tag{6}$$

where $\sigma(z)$ and $\tilde\sigma(z)$ are polynomials, mostly of second order, and $\tilde\tau(z)$ is a first-order polynomial. By separating of variables and applying following assumption

$$\psi_n(z) = \phi(z)y_n(z)\,, \tag{7}$$

Equation (6) reduces to following differential equations

$$\sigma y'' + \tau y' + \lambda y = 0\,, \tag{8}$$

$$\frac{\phi(z)'}{\phi(z)} = \frac{\tau(z)}{\sigma(z)}\,. \tag{9}$$

The function $y(z)$ is of the hypergeometric type which its polynomial representations can be obtained using following Rodrigues relation[32]

$$y_n(z) = \frac{C_n}{\rho(z)}\frac{{\rm d}^n}{{\rm d}z^n}[\sigma(z)^n\rho(z)]\,, \tag{10}$$

where C_n is the normalization coefficient. In order to solve Eq. (9), the functions $\rho(z)$, $\pi(z)$, and $\tau(z)$ should be determined by means of following known functions $\sigma(z)$, $\tilde\sigma(z)$, and $\tilde\tau(z)$ as,

$$\tau(z) = \tilde\tau(z) + 2\pi(z)\,, \tag{11}$$

$$(\sigma\rho)' = \tau\rho\,, \tag{12}$$

$$\pi = \frac{\sigma' - \tilde\tau}{2} \pm \sqrt{\Big(\frac{\sigma'-\tilde\tau}{2}\Big)^2 - \tilde\sigma + k\sigma}\,, \tag{13}$$

$$\lambda = k + \pi'\,, \tag{14}$$

$$\lambda = \lambda_n = -n\tau' - \frac{n(n+1)}{2}\sigma''\,, \quad n = 0,1,2,\ldots\,, \tag{15}$$

where τ' has negative values and k is a constant and can be determined such that the square root in Eq. (13) becomes positive.

3 Solutions of Schrödinger Equation for Single Nucleon

In this section, we employ the NU method to obtain energy eigenvalues and eigenfunctions of the neutron single particle. The Schrödinger equation for a single neutron (Eq. (2)) with complicated form of nuclear potential including the Woods–Saxon potential, spin-orbit interaction and centrifugal terms can be written as

$$\begin{aligned}\frac{{\rm d}^2R(r)}{{\rm d}r^2} + \frac{2m}{\hbar^2}\Big[E &- \frac{-V_0}{1+{\rm e}^{(r-R_0)/a}} \\ &- \frac{1}{2}V_{\rm LS}^{(0)} r_0^2 \frac{1}{r}\Big(\frac{\rm d}{{\rm d}r}\frac{1}{1+{\rm e}^{(r-R_0)/a}}\Big) \\ &\times\Big(j(j+1) - l(l+1) - \frac{3}{4}\Big) \\ &- \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\Big]R(r) = 0\,.\end{aligned} \tag{16}$$

In order to solve this complicated differential equation, it is necessary to introduce new variables and make some approximations. If l is not too large, the approximate expansion of the centrifugal potential $l(l+1)/r^2$ as function of Woods–Saxon potential near $r = r_m$, the minimum point of $V(r)$ (Eq. (5)), is reasonable and can be replaced by centrifugal potential in Schrödinger equation (Eq. (16)). This approximate expansion is given as

$$\begin{aligned}\frac{l(l+1)}{r^2} \approx \frac{l(l+1)}{r_m^2}\Big[C_0 &+ C_1\Big(\frac{-{\rm e}^{-\alpha r}}{1+q\,{\rm e}^{-\alpha r}}\Big) \\ &+ C_2\Big(\frac{-{\rm e}^{-\alpha r}}{1+q\,{\rm e}^{-\alpha r}}\Big)^2\Big]\,,\end{aligned} \tag{17}$$

where Woods–Saxon potential has been written as $-{\rm e}^{-\alpha r}/(1+q\,{\rm e}^{-\alpha r})$ and $\alpha = 1/a$, $q = {\rm e}^{\alpha R_0}$. The coefficients C_0, C_1, and C_2 are three constants as function of potential parameters, q, and l-dependent minimum point r_m. This approximate expansion has been widely used for different potentials,[17,33–35] and its accuracy and efficiency in comparison with other approximations for centrifugal potential form has been discussed in Refs. [35–36]. These coefficients can be derived explicitly. The details of derivation of Eq. (17) and its coefficients have been represented in Appendix.

By introducing new variable $z = -\,\mathrm{e}^{-\alpha r}$, constants $V_0' = V_0 q$, $V_{\rm LS}'^{0} = V_{\rm LS}^{0} q$, and using the approximation $1/r = (1/r_0')\,\mathrm{e}^{-\alpha r}$ (where r_0' is an adjustable parameter with dimension of length) and Eq. (17) for centrifugal term, the radial Schrödinger equation (Eq. (16)) is transformed to the following analytically solvable form

$$\begin{aligned} & z^2\frac{\mathrm{d}^2R(z)}{\mathrm{d}z^2} + z\frac{\mathrm{d}R(z)}{\mathrm{d}z} + \frac{2m}{\hbar^2}\Big[E - V_0'\Big(\frac{z}{1-qz}\Big) \\ & + \frac{\alpha r_0^2 V_{\rm LS}'^{(0)}}{2r_0'^2}\Big(j(j+1) - l(l+1) - \frac{3}{4}\Big)\Big(\frac{z}{1-qz}\Big)^2 \\ & - \frac{\hbar^2}{2m}\frac{l(l+1)}{r_m^2}\Big(C_0 + C_1\Big(\frac{z}{1-qz}\Big) \\ & + C_2\Big(\frac{z}{1-qz}\Big)^2\Big)\Big]R(z) = 0\,. \end{aligned} \tag{18}$$

By defining the three constants ε, β, and γ

$$\begin{aligned} \varepsilon &= \sqrt{\frac{l(l+1)}{\alpha^2 r_m^2}C_0 - \frac{2mE}{\hbar^2\alpha^2}}\,, \\ \beta &= 2q\varepsilon^2 - \frac{2mV_0'}{\hbar^2\alpha^2} - \frac{l(l+1)}{\alpha^2 r_m^2}C_1\,, \\ \gamma &= q^2\varepsilon^2 - \frac{2mqV_0'}{\hbar^2\alpha^2} - \frac{l(l+1)}{\alpha^2 r_m^2}(qC_1 - C_2) \\ & \quad - \frac{mV_{\rm LS}^{(0)} r^2_{\prime 0}}{\hbar^2\alpha r_0'}\Big(j(j+1) - l(l+1) - \frac{3}{4}\Big)\,, \end{aligned} \tag{19}$$

Eq. (18), reduces to the NU differential equation type

$$\begin{aligned} & \frac{\mathrm{d}^2R(z)}{\mathrm{d}z^2} + \frac{(1-qz)}{z(1-qz)}\frac{\mathrm{d}R(z)}{\mathrm{d}z} \\ & + \frac{(-\gamma z^2 + \beta z - \varepsilon^2)}{[z(1-qz)]^2}R(z) = 0\,. \end{aligned} \tag{20}$$

By comparing this equation with standard form of NU equation (Eq. (6)), the parameters of NU equation are derived as

$$\begin{aligned} & \tilde{\tau}(z) = (1-qz)\,, \quad \sigma(z) = z(1-qz)\,, \\ & \tilde{\sigma}(z) = -\gamma z^2 + \beta z - \varepsilon^2\,. \end{aligned} \tag{21}$$

These parameters can be used to determine two functions $\pi(z)$, $\tau(z)$, and constant k

$$\pi(z) = \varepsilon - \frac{q}{2}(1 + 2\varepsilon + S)z\,, \tag{22}$$

$$k = \beta - (2\varepsilon + S)q\varepsilon\,, \tag{23}$$

$$\tau(z) = 1 + 2\varepsilon - q(2 + 2\varepsilon + S)z\,, \tag{24}$$

where

$$S = \sqrt{1 + \frac{4l(l+1)}{q^2\alpha^2 r_m^2}C_2 - \frac{4mV_{\rm LS}'^{(0)} r_0^2}{q^2\hbar^2\alpha r_0'}\Big(j(j+1) - l(l+1) - \frac{3}{4}\Big)}\,. \tag{25}$$

By substituting the relations of $\pi'(z)$, $\tau'(z)$, $\sigma''(z)$, and k in Eqs. (14) and (15), the dimensionless parameter ε is obtained as a function of quantum numbers n, l, and j

$$\varepsilon_{nlj} = -\Big[\frac{2mV_0/\hbar^2\alpha^2 + l(l+1)C_1/q\alpha^2 r_m^2 + (n^2 + (n+1/2)(1+S_{jl}))}{(1 + 2n + S_{jl})}\Big]\,. \tag{27}$$

Hence by means of above equation the energy eigenvalues $E = \hbar^2 l(l+1)C_0/2mr_m^2 - (\hbar^2/2ma^2)\varepsilon^2$ is obtained explicitly as:

$$E_{nlj} = \frac{\hbar^2 l(l+1)C_0}{2mr_m^2} - \frac{\hbar^2}{2ma^2}\Big[\frac{2ma^2V_0/\hbar^2 + l(l+1)a^2C_1/qr_m^2 + (n^2 + (n+1/2)(1+S_{jl}))}{(1 + 2n + S_{jl})}\Big]^2\,.$$

This energy eigenvalue which has been derived for any arbitrary quantum numbers n, l, and j indicates the bound state structure of single neutron in nuclei. This equation without spin-orbit interaction term reduces to Eq. (58) in Ref. [17].

In order to obtain the corresponding eigenfunctions, the functions $\rho(z)$ and $\phi(z)$ are evaluated using functions $\sigma(z)$, $\pi(z)$ and $\tau(z)$. Through Eqs. (9) and (12)

$$\rho(z) = (1-qz)^{S_{jl}} z^{2\varepsilon_{nlj}}\,, \tag{28}$$

$$\phi(z) = (1-qz)^{(1/2)(1+S_{jl})} z^{\varepsilon_{nlj}}\,. \tag{29}$$

By substituting $\rho(z)$ and $\sigma(z)$ in Eq. (10), the hypergeometric-type solution $y(z)$ is derived by multiplication of $y(z)$ and $\phi(z)$, as Eq. (7), the neutron single particle reduced radial wave function can be obtained as

$$\begin{aligned} R_{nlj}(z) &= N_{nlj}(1-qz)^{(1/2)(1-S_{jl})} \\ & \quad \times z^{-\varepsilon_{nlj}}\frac{\mathrm{d}^n}{\mathrm{d}z^n}[(1-qz)^{(n+S_{jl})} z^{n+2\varepsilon_{nlj}}]\,, \end{aligned} \tag{30}$$

where N is the normalization constant. Therefore the analytic radial wave function of single neutron in presence of Woods–Saxon nuclear potential, spin-orbit interaction and centrifugal potential in terms of variable $z(r) = -q\,\mathrm{e}^{-r/a}$, hypergeometric function F can be written as

$$\begin{aligned} \psi_{nlj}(r) &= N_{nlj}\frac{1}{r}z^{\varepsilon_{nlj}}(1-qz)^{(1/2)(1+S_{jl})} \\ & \quad {}_2F_1(-n, 1 + 2\varepsilon_{nlj} + S_{jl} + n; 2\varepsilon_{nlj} + 1; qz)\,. \end{aligned} \tag{31}$$

4 Conclusion

In this theoretical investigation, the radial Schrödinger equation for a single neutron has been solved analytically for complicated potentials consist of Woods–Saxon potential, spin-orbit interaction, and centrifugal terms, by NU method. By using approximate expansion of $1/r^2$ in terms of Woods–Saxon type function, which its details have been represented in Appendix, the Schrödinger equation has been transformed to the analytically solvable differential equation of NU equation. By means of NU method, and introducing some new variables and constants the energy eigenvalue and corresponding wave function of single neutron, as an example of single nucleon problem, have been derived analytically. The obtained results at special case which spin-orbit interactions did not take into account, are reduced to the theoretical results of published papers (as example Ref. [17]). This method also can be used for proton single-particle and it is capable to give the analytic solution of single nucleon for both proton and neutron, by adding the coulomb potential to the total potentials. The analytic solution of single nucleon Schrödinger equation with Woods–Saxon basis, for any arbitrary n, l, and j, can be used for theoretical analysis of mean-field shell model, including single nucleon energy levels and wave functions, the particle-hole theory, electromagnetic transitions, and study of nuclear reactions and scattering.

Appendix

In order to find the coefficients of Eq. (17), after introducing a new exponential variable the right hand side (R.H.S) and left hand side (L.H.S) of this equation are expanded about the l-dependent minimum point r_m, separately. Clearly this exponential variable can be different and should be determined according to the form of potential and therefore the coefficients would not be same in different cases.

By introducing exponential variable $z = -\,\mathrm{e}^{-\alpha r}$, L.H.S ($f(z) = \alpha^2/\ln^2(-z)$) can be expanded in a Taylor series around z_l, ($z_l = -\,\mathrm{e}^{-\alpha r_m}$), as

$$f(z) = \frac{\alpha^2}{\ln^2(-z_l)} + \Big(\frac{-2\alpha^2}{z_l \ln^3(-z_l)}\Big)(\Delta z) + \Big(\frac{\alpha^2(3+\ln(-z_l))}{z_l^2 \ln^4(-z_l)}\Big)\frac{(\Delta z)^2}{2!} + O(\Delta z^3)\,, \tag{A1}$$

where $\Delta z = (z - z_l)$.

The R.H.S with this new variable, i.e. $f(z) = C_0' + C_1'(z/(1-qz)) + C_2'(z/(1-qz))^2$, can be transformed to the form of the above equation, by expanding its terms, $f_1(z) = (z/(1-qz))$ and $f_2(z) = (z/(1-qz))^2$ around z_l and can be written as

$$\begin{aligned} f(z) = {} & \Big[C_0' + \frac{z_l C_1'}{(1-qz_l)} + \frac{z_l^2 C_2'}{(1-qz_l)^2}\Big] + \Big[\frac{(2C_2' - qC_1')z_l + C_1'}{(1-qz_l)^3}\Big](\Delta z) \\ & + 2\Big[\frac{(2qC_2' - C_1')z_l + (C_1' q + C_2')}{(1-qz_l)^4}\Big]\frac{(\Delta z)^2}{2!} + O(\Delta z^3)\,. \end{aligned} \tag{A2}$$

By equating two Eqs. (A1) and (A2) and terms of the same power up to second order of the $\Delta z = z - z_l$, a set of equations is derived which can be solved simplicity and the coefficients are obtained explicitly as

$$\begin{aligned} C_0' &= t_1 + \Big(\frac{m_{13}m_{32} - m_{12}m_{33}}{m_{22}m_{33} - m_{23}m_{32}}\Big)t_2 + \Big(\frac{m_{12}m_{23} - m_{13}m_{22}}{m_{22}m_{33} - m_{23}m_{32}}\Big)t_3\,, \\ C_1' &= \Big(\frac{m_{33}}{m_{22}m_{33} - m_{23}m_{32}}\Big)t_2 + \Big(\frac{-m_{23}}{m_{22}m_{33} - m_{23}m_{32}}\Big)t_3\,, \\ C_2' &= \Big(\frac{-m_{32}}{m_{22}m_{33} - m_{23}m_{32}}\Big)t_2 + \Big(\frac{m_{22}}{m_{22}m_{33} - m_{23}m_{32}}\Big)t_3\,, \end{aligned} \tag{A3}$$

where

$$m_{12} = \frac{z_l}{1-qz_l}\,, \quad m_{13} = m_{12}^2\,, \quad m_{22} = \frac{1}{(1-qz_l)^2}\,, \quad m_{23} = 2m_{12}m_{22}\,, \quad m_{32} = \frac{q - z_l}{(1-qz_l)^4}\,,$$

$$m_{33} = \frac{1+2qz_l}{(1-qz_l)^4}\,, \quad t_1 = \frac{\alpha^2}{\ln^2(-z_l)}\,, \quad t_2 = \frac{-2\alpha^2}{z_l \ln^3(-z_l)}\,, \quad t_3 = \frac{\alpha^2(3+\ln(-z_l))}{z_l^2 \ln^4(-z_l)}\,.$$

The coefficients for $q = 1$ reduces to the well known form of

$$\begin{aligned} C_0' &= \frac{1}{r_m^2}\Big[1 - \frac{(1+\mathrm{e}^{-\alpha r_m})^2}{\alpha^2 r_m^2}\Big(\frac{4\alpha r_m}{1+\mathrm{e}^{-\alpha r_m}} - 3 - \alpha r_m\Big)\Big]\,, \\ C_1' &= \frac{1}{r_m^2}\Big[-2(1+\mathrm{e}^{\alpha r_m})\Big(3\Big(\frac{1+\mathrm{e}^{-\alpha r_m}}{\alpha r_m}\Big) - (3+\alpha r_m)\Big(\frac{1+\mathrm{e}^{-\alpha r_m}}{\alpha r_m}\Big)^2\Big)\Big]\,, \\ C_2' &= \frac{1}{r_m^2}[(1+\mathrm{e}^{\alpha r_m}\Big)^2\Big(\frac{1+\mathrm{e}^{-\alpha r_m}}{\alpha r_m}\Big)^2\Big(3 + \alpha r_m - \frac{2\alpha r_m}{1+\mathrm{e}^{-\alpha r_m}}\Big)\Big]\,. \end{aligned} \tag{A4}$$

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