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Numerical–Fitting–Nikiforov–Uvarov method applied to Schrödinger Equation

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Abstract In this work, we have solved the radial Schrödinger equation for the Woods–Saxon potential together with coulomb (r>Rc), centrifugal terms and spin-orbit interaction by using a new type of Nikiforov-Uvarov (NU) method. This approach is based on the Second-Order Linear Differential Equations (SOLDE) solution. The mandatory specific choices of the required parameters in this technique restrict the application of this method to the Schrödinger equation with complicated potential profiles, which means that the NU method cannot efficiently be employed to solve more realistic physical systems. Due to the mentioned difficulties in evaluating the equivalent second-order algebraic equation in the NU method, the analytical NU method has to be extended to the more efficient version combined with numerical methods (that leads to a semi-analytical method). We have solved it by combining the NU method with the numerical fitting schema. The numerical fitting schema helps us find the mentioned second-order algebraic equation. Otherwise, complicated changes of variables or overwhelming algebraic treatments to derive the energy eigenvalues and the wavefunctions are required. The current approach is simpler, more flexible and efficient. This technique can also be developed for equations other than the Schrodinger one. The Woods–Saxon potential is also a short-range interaction in the potential model for nuclear physics and has predictions for the nuclear shell model and distribution of nuclear densities. We have obtained semi-analytical energy eigenvalues and eigenfunctions for various values of n, l, and j quantum numbers. Agreement of $5/2^+$ and $1/2^+$ wavefunctions with the published works is also obtained, showing the accuracy of our method.

1 Introduction

The asymptotic giant branch [1] is an evolutionary phase through which many stars, including the Sun, eventually pass. This phase involves a hydrogen and a helium shell that burns alternately, surrounding an inactive stellar core. The ^{16}O(p, γ)^{17}F reaction rate sensitively influences the ^{17}O/16O isotope predicted by models of massive stars, where proton captures occur at the base of the convective envelope. In the study of the breakup of ^{17}F into proton + ^{16}O, some potential models for 17F have been used previously, such as Woods–Saxon Potential with Spin-Orbit and Coulomb potentials [2] and M3Y interaction model [3]. The solution of the Schrödinger equation, including the above potentials, has been done using the numerical methods in the above-mentioned works. This is because the analytical solution of these equations is not possible. However, some theoretical groups have tried to solve these Schrödinger equations analytically. For example, Pahlavani et al. solved the Schrödinger equation, including Woods–Saxon Potential with Spin-Orbit and Centrifugal Terms by Nikiforov–Uvarov Method [4]. They did not include the coulomb term in their calculations. Adding the coulomb potential (here for r<Rc; Rc= spherical nucleus radius) and the solution of the Schrödinger equation by the Nikiforov–Uvarov Method is the main goal of the present work. Our previous works used the NU method to solve the Schrödinger equation with different potentials. Energy-dependent potential [5] and angle-dependent potential [6] are two. We have also solved the Dirac equation with the NU method, including Hartmann Potential [7], Duffin–Kemmer–Petiau (DKP) equation with Woods–Saxon Potential [8] and Hulthen vector potential [9] and Klein–Gordon equation with Energy-Dependent Potential [10]. We have solved the Schrödinger equation in the presence of the spin-orbit interaction, Woods–Saxon potential together with coulomb (r>Rc) and centrifugal terms by a combination of the numerical fitting and NU methods and obtained energy eigenvalues and corresponding eigenfunctions.

2 Parametric NU method

This powerful mathematical tool could be used to solve

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the second-order differential equations. Considering the following differential equation [10–12]

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

Where $\sigma(z)$ and $\tilde{\sigma}(z)$ are polynomials of second order at most, and $\tilde{\tau}(z)$ is a first-order polynomial. To make the application of the NU method simpler and the checking of the validity of the solution unnecessary, we present a shortcut for the method. We begin the method by writing the general form of the Schrodinger-like equation (1) as

$$\psi_n''(s)+\left(\frac{c_1-c_2s}{s(1-c_3s)}\right)\psi_n'(s)+\left(\frac{-p_2s^2+p_1s-p_0}{s^2(1-c_3s)^2}\right)\psi_n(s)=0, \tag{2}$$

where the wave functions satisfy

$$\psi_n(s)=\phi(s)y_n(s). \tag{3}$$

By comparing Eq. (3) with its counterpart Eq. (2), one can obtain

$$\tilde{\tau}(s)=c_1-c_2s,\qquad \sigma(s)=s(1-c_3s),\quad \tilde{\sigma}(s)=-p_2s^2+p_1s-p_0, \tag{4}$$

According to the NU method [10], one can obtain the bound state energy equation as [11, 12]

$$c_2n-(2n+1)c_5+(2n+1)\left(\sqrt{c_9}+c_3\sqrt{c_8}\right)+n(n-1)c_3+c_7+2c_3c_8+2\sqrt{c_8c_9}=0, \tag{5}$$

where,

$$c_4=\frac{1}{2}(1-c_1), \tag{6-1}$$

$$c_5=\frac{1}{2}(c_2-2c_3), \tag{6-2}$$

$$c_6=c_5^2+p_2, \tag{6-3}$$

$$c_7=2c_4c_5-p_1, \tag{6-4}$$

$$c_8=c_4^2+p_0, \tag{6-5}$$

$$c_9=c_3(c_7+c_3c_8)+c_6, \tag{6-6}$$

$$c_4=\frac{1}{2}(1-c_1). \tag{6-7}$$

In addition, we also find that:

$$\rho(s)=s^{c_{10}}(1-c_3s)^{c_{11}}, \tag{7-1}$$

$$\varphi(s)=s^{c_{12}}(1-c_3s)^{c_{13}}, \tag{7-2}$$

$$c_{12}>0, c_{13}>0, \tag{7-3}$$

$$y_n(s)=P_n^{(c_{10},c_{11})}(1-2c_3s), c_{10}>-1, c_{11}>1, \tag{7-4}$$

are necessary in calculating the wave functions.

$$\psi_{nl}(s)=N_{nl}s^{c_{12}}(1-c_3s)^{c_{13}}P_n^{(c_{10},c_{11})}(1-2c_3s), \tag{8}$$

where, $P_n^{(\mu,\nu)}(x), \mu>1, \nu>1, x\in[-1,1]$ are Jacobi polynomials. All undefined constant parameters are as follows [13],

$$c_{10}=c_1+2c_4+2\sqrt{c_8}, \tag{9-1}$$

$$c_{11}=1-c_1-2c_4+\frac{2}{c_2}\sqrt{c_9}, \tag{9-2}$$

$$c_{12}=c_4+\sqrt{c_8}, \tag{9-3}$$

$$c_{13}=-c_4+\frac{1}{c_3}\left(\sqrt{c_9}+c_5\right), \tag{9-4}$$

where $c_3\neq 0$, $c_{13}>0$, $c_{12}>0$, $s\in\left[\frac{1,1}{c_{13}}\right]$ and $c_{13}\neq 0$.

3 Solutions of Schrödinger Equation

We start with the radial part of the Schrödinger equation as,

$$\frac{d^2R(r)}{dr^2}+\frac{2\mu}{\hbar^2}\left[E-V(r)-\frac{\hbar^2 l(l+1)}{2\mu r^2}\right]R(r)=0. \tag{10}$$

The potential profile contains the following terms:
1- woods-saxon term:

$$V_{WS}=\frac{-V_0}{1+e^{\frac{(r-R_0)}{a}}}, \tag{11}$$

were we have used $V_0=42.77MeV$ for ^{17}F atoms.
2- spin-orbit term:

$$V_{LS}(r)=\frac{1}{2}V_{LS}^{(0)}\left(\frac{r_0}{\hbar}\right)^2\frac{1}{r}\left[\frac{d}{dr}\frac{1}{1+e^{\frac{(r-R_0)}{a}}}\right](\vec{L}.\vec{S}), \tag{12}$$

where we have used $V_{LS}^{(0)}=0.44V_0$.
3- Coulomb term:

$$V_C(r)=\begin{cases}\dfrac{e^2}{\pi\varepsilon_0 R_C}\left[3-\left(\dfrac{r}{R_C}\right)^2\right] & r\le R_C\\ \dfrac{8e^2}{4\pi\varepsilon_0 r} & r>R_C\end{cases}\quad . \qquad (13)$$

Here we have solved the Schrödinger equation for $r>R_c$. By using the change of variable as $\psi(r)=rR(r)$ we have,

$$\frac{d\psi}{dr}=R(r)+r\frac{dR(r)}{dr}. \qquad (14)$$

Then the Schrödinger equation becomes

$$\frac{d^2\psi(r)}{dr^2}+\frac{2\mu E}{\hbar^2}\psi(r)-\frac{2\mu V(r)}{\hbar^2}\psi(r)-\frac{l(l+1)}{r^2}\psi(r)=0. \qquad (15)$$

Now, the complete Schrödinger equation reads,

$$\frac{d^2\psi(r)}{dr^2}+\frac{2\mu}{\hbar^2}\Bigg[E-\frac{-V_0}{1+e^{\frac{(r-R_0)}{a}}} -\frac{1}{2}V_{LS}^{(0)}r_0^2\frac{1}{r}\left(\frac{d}{dr}\frac{1}{1+e^{\frac{(r-R_0)}{a}}}\right)\left(j(j+1)-l(l+1)-\frac{3}{4}\right) -\frac{1}{4\pi\varepsilon_0}\frac{8e^2}{r}\Bigg]\psi(r)-\frac{l(l+1)}{r^2}\psi(r)=0. \qquad (16)$$

We need another change of variable, which leads to

$$\frac{d\psi(r)}{dr}=\frac{d\psi(r)}{ds}\times\frac{ds}{dr}=-\delta s\frac{d\psi(r)}{ds}, \qquad (17-1)$$

$$\frac{d^2\psi(r)}{dr^2}=\delta^2 s^2\frac{d^2R(s\quad)}{ds^2}+\delta^2 s\frac{dR(s\quad)}{ds}. \qquad (17-2)$$

We define $\delta=\frac{1}{a}$, $q=e^{\delta R_0}$, $V_0^{'}=V_0q$ and $V_{LS}^{'0}=V_{LS}^0q$. We have also used the following approximation:

$$\frac{1}{r^2}\approx\delta^2\left(\frac{e^{-\delta r}}{1-e^{-\delta r}}\right)^2. \qquad (18)$$

To find the best value of the δ we have changed the δ and plotted both side of the above equation several times and found the best δ to be 0.4fm^{-1}. Figure (1) shows two sides of the above equation to obtain δ. By using the later change of variable, the Schrödinger equation reads,

$$\delta^2 s^2\frac{d^2R(s)}{ds^2}+\delta^2 s\frac{dR(s)}{ds}+\left(\frac{2\mu E}{\hbar^2}+\frac{2\mu V_0'}{\hbar^2}\right)\left(\frac{s}{1+qs}\right) +\frac{\mu\delta^2 r_0^2 V'^0_{LS}}{\hbar^2}\left(j(j+1)-l(l+1)-\frac{3}{4}\right)\frac{s^2}{(1-s)(1+qs)^2} -\frac{4\mu e^2\,\delta}{\pi\hbar^2\,\varepsilon_0}.\frac{s}{1-s}-l(l+1)\frac{\delta^2 s^2}{(1-s)\verb|^|2\,)}R(s)=0. \qquad (19)$$

After some simplifications we have

$$\frac{d^2R(s)}{ds^2}+\frac{1}{s}\frac{dR(s)}{ds}+\left(\frac{\frac{2\mu E}{(\hbar^2\delta^2)(1-s)^2}+\frac{2\mu V_0'}{\hbar^2\delta^2}\frac{s(1-s)^2}{(1+qs)}}{s^2(1-s)^2} +\frac{\frac{\mu r_0^2 V'^0_{LS}}{\hbar^2}\left(j(j+1)-l(l+1)-\frac{3}{4}\right)\frac{s^2(1-s\quad)}{(1+qs)^2}}{s^2(1-s)^2} -\frac{\frac{4\mu e^2}{\pi\varepsilon_0\hbar^2\delta}s(\,1-s\quad)-l(l+1)s^2}{s^2(1-s)^2}\right)R(s)=0. \qquad (20)$$

In order to use the N-U method we have to convert the numerator of the potential term to a second order polynomial For this purpose, we have used the following approximations,

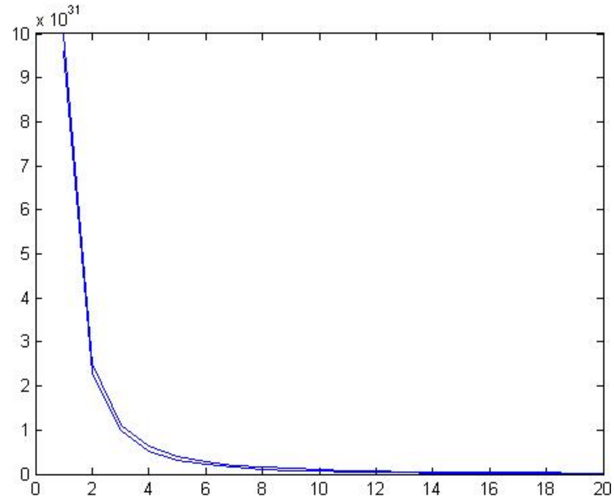

Fig. 1 Left hand side and Right hand side of the equation (3-1) to obtain δ .

$$\frac{s(1-s[\![\;)^2]\!]}{1+qs}=0.006595579s^2-\ 0.0132710857s+\ 0.0067413175, \qquad (21)$$

which has been obtained through numerical fitting schema. Figure (2) shows the two sides of the equation above.

As it is clear, this approximation is extremely good. We have also used from:

$$\frac{s^2(1-s\quad)}{(1+qs)^2}=-3.3579988\times10^{-9}s^2-0.432019240084\times10^{-4}s+0.4341808999\times10^{-4}, \qquad (22)$$

which has been obtained through numerical fitting schema. Figure (3) shows the two sides of the equation above.

As it is clear, this approximation is extremely good. In order to convert the last Schrödinger equation to the N-U type Schrödinger equation,

$$\psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s) + \frac{\tilde{\sigma}(s)}{\sigma(s)^2}\psi_n(s) = 0, \quad (23)$$

$$\psi_n''(s) + \left(\frac{1-s}{s(1-s)}\right)\psi_n'(s) + \left(\frac{-\gamma s^2 + \beta s - \varepsilon^2}{s^2(1-s)^2}\right)\psi_n(s) = 0, \quad (24)$$

We define three parameters $\varepsilon, \beta, \gamma$ as follows,

$$-\gamma = \frac{2\mu E}{\hbar^2\delta^2} + \frac{2\mu V_0'}{\hbar^2\delta^2}(0.006595579) - \left(\frac{\mu V'^{(0)}_{LS} r_0^2\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{\hbar^2}\right) \times 3.3579988 \times 10^{-9} + \frac{4\mu e^2}{\pi\varepsilon_0\hbar^2\delta} - l(l+1), \quad (25-1)$$

$$\beta = -\frac{4\mu E}{\hbar^2\delta^2} - \frac{2\mu V_0'}{\hbar^2\delta^2}(0.0132710857) - \frac{\mu V'^{(0)}_{LS} r_0^2\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{\hbar^2} \times (0.432019240084 \times 10^{-4}) - \frac{4\mu e^2}{\pi\varepsilon_0\hbar^2\delta}. \quad (25-2)$$

Now we write the β,γ as function of ε:

$$-\gamma = \frac{2\mu E}{\hbar^2\delta^2} + \frac{2\mu V_0'}{\hbar^2\delta^2}(0.006595579) - \frac{\mu V'^{(0)}_{LS} r_0^2\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{\hbar^2} \times (3.3579988.10^{-9}) + \frac{4\mu e^2}{\pi\varepsilon_0\hbar^2\,\delta} - l(l+1), \quad (26-1)$$

$$\beta = -\frac{4\mu E}{\hbar^2\delta^2} - \frac{2\mu V_0'}{\hbar^2\delta^2}(0.0132710857) - \frac{\mu V'^{(0)}_{LS} r_0^2\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{\hbar^2} \times (0.432019240084.10^{-4}) - \frac{4\mu e^2}{\pi\varepsilon_0\hbar^2\,\delta}, \quad (26-2)$$

$$-\varepsilon^2 = \frac{2\mu E}{\hbar^2\delta^2} + \frac{2\mu V_0'}{\hbar^2\delta^2}(0.0067413175) + \frac{\mu V'^{(0)}_{LS} r_0^2\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{\hbar^2} \times (0.4341808999.10^{-4}). \quad (26-3)$$

Now we write the β, γ as function of ε,

$$\gamma = \varepsilon^2 + \frac{\mu V_0'}{\hbar^2\delta^2}(0.000291477) + \frac{\mu V'^{(0)}_{LS} r_0^2\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{\hbar^2} \times (0.434214479888 \times 10^{-4}) - \frac{4\mu e^2}{\pi\varepsilon_0\hbar^2\delta} + l(l+1) \rightarrow \gamma = \varepsilon^2 + A, \quad (27-1)$$

$$\beta = 2\varepsilon^2 + \frac{\mu V_0'}{\hbar^2\delta^2}(0.0004230986) + \frac{\mu V'^{(0)}_{LS} r_0^2\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{\hbar^2} \times (0.436342559716 \times 10^{-4}) - \frac{4\mu e^2}{\pi\varepsilon_0\hbar^2\delta} \rightarrow \beta = 2\varepsilon^2 + B, \quad (27-2)$$

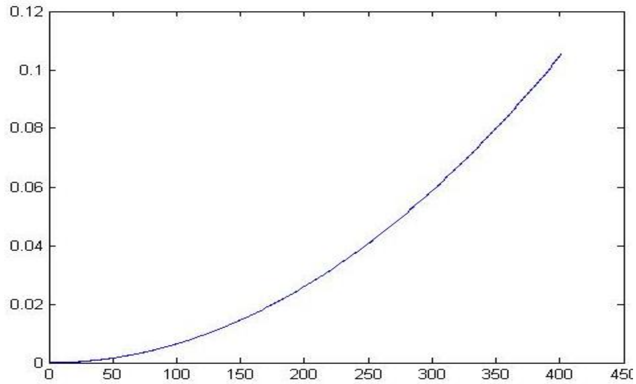

Fig. 2 left hand side and right-hand side of the equation (3-2) to show the accuracy of this approximation.

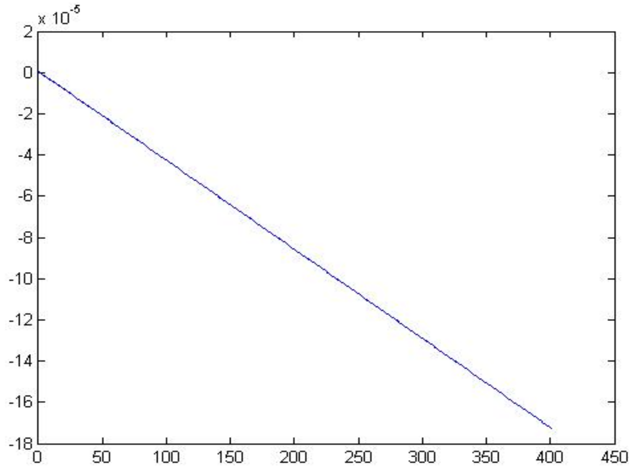

Fig. 3 Left hand side and right hand side of the equation (3-3) to show the accuracy of this approximation

Based on what we have described above in the N-U section, we can find the following second order polynomial,

$$\mathrm{n}-(2\,\mathrm{n}+1)\left(-\frac{1}{2}\right)+(2\,\mathrm{n}+1)\left(\sqrt{\gamma-\beta+\varepsilon^2+\frac{1}{4}}+\varepsilon\right)$$
$$+\,\mathrm{n}(\,\mathrm{n}+1)-\beta+2\varepsilon^2+2\varepsilon\sqrt{\gamma-\beta+\varepsilon^2+\frac{1}{4}}$$
$$=0, \qquad (28)$$

After some simplifications we have,

$$\left[4\left(A-B+\frac{1}{4}\right)-(2\,\mathrm{n}+1)^2\right]\varepsilon^2$$
$$+2(2\mathrm{n}+1)[2\mathrm{A}-\mathrm{B}-\mathrm{n}^2-\mathrm{n}]\varepsilon$$
$$+\left[(2\,\mathrm{n}+1)^2\left(\mathrm{A}-\mathrm{B}+\frac{1}{4}\right)-\left(n^2+n+\frac{1}{2}-B\right)^2\right]$$
$$=0, \qquad (29-1)$$

$$h_2\varepsilon^2+h_1\varepsilon+h_0=0. \qquad (29-2)$$

By solving this equation and obtaining the $\mathcal{E}$ we will wined the energies E as,

$$\mathrm{E_{nlj}}=(-(\hbar\text{^}2\ \delta\text{^}2)/2\mu)(\varepsilon^2+\frac{2\mu V_0^{'}}{(\hbar^2\delta^2)(0.0067413175)}$$
$$+\frac{\mu V'^{(0)}_{LS}\,\mathrm{r}_0^2\left(\mathrm{j}(\mathrm{j}+1)-\mathrm{l}(\mathrm{l}+1)-\frac{3}{4}\right)}{\hbar^2}$$
$$\times(0.4341808999\times10^{-4}). \qquad (30)$$

Ground state energy of the ^{17}F can be obtained by using of $j=\frac{5}{2}$, n = 0 , l =2 and the first excited states can be calculated by using of the $j=\frac{1}{2}$, n = 1 , l = 0 . Now, the wave-functions can be obtained through,

$$\psi(\mathrm{s})=\mathrm{y}(\mathrm{s})\phi(\mathrm{s}), \qquad (31-1)$$

$$\rho(\mathrm{s})=\mathrm{s}^{1+2\varepsilon}(1-\mathrm{s})^{2\sqrt{\gamma-\beta+\varepsilon^2+\frac{1}{4}}}, \qquad (31-2)$$

$$\phi(\mathrm{s})=\mathrm{s}^{\varepsilon}(1-\mathrm{s})^{\left(\sqrt{\gamma-\beta+\varepsilon^2+\frac{1}{4}}-\frac{1}{2}\right)}, \qquad (31-3)$$

$$\mathrm{y_n}(\mathrm{s})=\mathrm{P_n}^{\left(1+2\varepsilon,2\sqrt{\gamma-\beta+\varepsilon^2+\frac{1}{4}}\right)}(1-2\mathrm{s}), \qquad (31-4)$$

$$\psi_{\mathrm{nl}}(\mathrm{s})=\mathrm{N_{nl}}\mathrm{s}^{\varepsilon}(1-\mathrm{s})^{\sqrt{\gamma-\beta+\varepsilon^2+\frac{1}{4}}+\frac{1}{2}}$$
$$\times\,\mathrm{P_n}^{\left(1+2\varepsilon,2\sqrt{\gamma-\beta+\varepsilon^2+\frac{1}{4}}\right)}(1-2\mathrm{s}), \qquad (31-5)$$

where $P_n^{(\mu,\nu)}(x),\mu>-1,\nu>-1,x\in[-1,1]$ are Jacobi polynomials. Ground state and first excited state wave functions are presented in the figures (4) and (5) respectively. As we can see in the figures (4-5), good agreement exists.

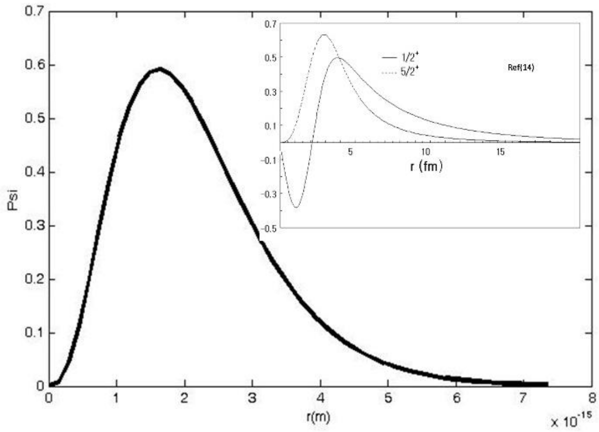

Fig. 4 – Normalized 5/2$^+$state wave function which we have calculated compared with ref [14] (inset panel) as a function of the radius r (fm)

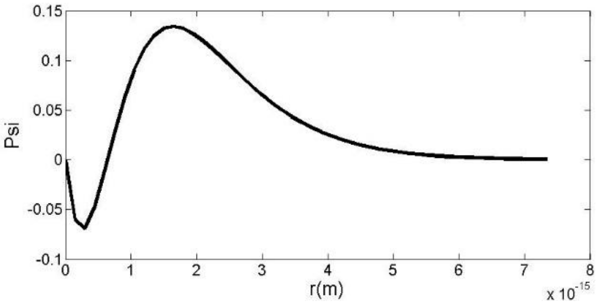

Fig. 5 – First excited state wave function by using of J=1/2$^+$. compare with ref [14] (inset panel of the figure 4)

Conclusions

In this study, the non-relativistic radial Schrödinger equation solved for Wood-Saxon potential together with coulomb potential (here for r>R_c; R_c= spherical nucleus radius), spin-orbit interaction and centrifugal term by a combination of the Nikiforov-Uvarov and numerical fitting methods. The energy eigen-functions and eigen-values of this model system obtained by NU method. For this purpose, by using approximate expansion of 1/r^2, as well was using equivalent second order algebraic equation in the NU method (a big difficulty in this method), the Schrödinger equation has been transformed to an analytically solvable differential equation. However, in a case study which one is not able to obtain an appropriate equivalent second order algebraic equation in the NU method, this method will not be applicable to that problem. By using this method, good agreement with previously published works values obtained.

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