INVESTIGATION OF NUCLEON SINGLE-PARTICLE ENERGY LEVELS IN ^{90}Zr USING NUMEROV METHOD

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Abstract

In this research work, nucleons single-particle energy levels of ^{90}Zr have been investigated by solving non-relativistic Schrödinger equation within the framework of Numerov method. In this calculation, phenomenological Wood-Saxon potential has been applied and Coulomb interaction is taken into account for proton state investigation. Due to the effect of Coulomb repulsion the single-particle energy levels of proton is higher than neutron. Moreover, ^{90}Zr permits the application of Hartree-Fock Random Phase Approximation RPA based Skyrme effective nucleon-nucleon interaction KDE0v1, BsK1, SIII, SVII and SGOI. So, the calculated results were compared with two set parameters of Skyrme interaction: BsK1, SVII and available experimental data. The results were agreed with these two parameters and experimental data.

Keywords: single-particle energy levels, Numerov method, ^{90}Zr

Introduction

The understanding of nuclear structure and energy levels of nuclei is important because it make an effort to study strong nuclear interaction between the nucleons that form a nucleus. The single-particle energies of a nucleon in the potential of the core, provide severe tests of nuclear model. The nuclear models are restored to find a wide range of nuclear properties and many nuclear models such as Fermi gas model, liquid drop model, single-particle shell model and cluster model have been introduced. Among them the single-particle shell model is one of the most essential models in order to make predictions and extrapolations for the properties of nuclei even further from stability (A. Signoracci and B. Alex Brown, 2007).

^{90}Zr is one of the medium mass nuclei with doubly closed shells where the number of neutrons is unequal to the number of protons. The nucleon single-particle energy levels of this nucleus can be investigated by using a self-consistent spherical Hartree-Fock HF method and Random Phase Approximation RPA with five different Skyrme type effective nucleon-nucleon interaction: KDE0v1, BsK1, SIII, SVII and SGOI. In the present work, we investigate single-particle energy levels of ^{90}Zr within the shell model approach using numerov method and compared with two sets parameters of Skyrme type effective nucleon-nucleon interaction BsK1, SVII and the available experimental data.

Numerov Method

Numerov method is a numerical method to solve second order differential equations. In this research work, the nucleon single-particle energies of *Zr* have been investigated within the framework of shell model approach and one body Schrödinger radial equation will be applied.

The Schrödinger radial equation can be represented by

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

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where $u(r) \equiv r R_{nl}$ is reduced radial wave function. A regular solution near the origin is $u(r \to 0) \to r^{l+1}$ and asymptotic solution is $u(r \to \infty) \to u(r) = e^{-\alpha r^2}$ where α is a constant. Now the Schrödinger equation becomes

$$\frac{d^2 u(r)}{d r^2} + k(r)\, u(r) = 0 \tag{2}$$

where $k(r) \equiv \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}\right]$ is the kernel of the equation, μ is mass of nucleon single particle and $V(r)$ is single nucleon potential. E.q (2) can be solved by means of Numerov Algorithm. In this method, the range *(r)* is split into N points according to the formula $r_n = r_{n+1} + h$ where h is the step. Then the wave function and kernel of the equation become $u_n \equiv u(r_n) = u(r_{n-1} + h)$ and $k_n \equiv k(r_n) = k(r_{n-1} + h)$. By using Taylor series, the reduced radial wave function $u(r)$ can be expand as

$$u_{n+1} \equiv u(r_n + h) = u(r_n) + h u'(r_n) + \frac{h^2}{2} u''(r_n) + \frac{h^3}{6} u'''(r_n) + \frac{h^4}{24} u^{(iv)}(r_n) + 0\left(h^5\right) \tag{3}$$

$$u_{n-1} \equiv u(r_n - h) = u(r_n) - h u'(r_n) + \frac{h^2}{2} u''(r_n) - \frac{h^3}{6} u'''(r_n) + \frac{h^4}{24} u^{(iv)}(r_n) + 0\left(h^5\right) \tag{4}$$

By adding Eq. (3) and (4), we get

$$u(r_n + h) = 2u(r_n) - u(r_n - h) - h^2 k(r_n)\, u(r_n) + \frac{h^4}{12} u^{(iv)}(r_n) \tag{5}$$

Similarly for the wave function with second-order derivative,

$$u''_{n+1} \equiv u''(r_n + h) = u''(r_n) + h u'''(r_n) + \frac{h^2}{2} u^{(iv)}(r_n) + \frac{h^3}{6} u^{(v)}(r_n) + 0\left(h^6\right) \tag{6}$$

$$u''_{n-1} \equiv u''(r_n - h) = u''(r_n) - h u''(r_n) + \frac{h^2}{2} u^{(iv)}(r_n) - \frac{h^3}{6} u^{(v)}(r_n) + 0\left(h^6\right) \tag{7}$$

According to the same operation of Eq. (3) and (4), we get

$$h^2 u^{(iv)}(r_n) = -k(r_{n+1})\, u(r_{n+1}) - k(r_{n-1})\, u(r_{n-1}) + 2k(r_n)\, u(r_n) \tag{8}$$

Substituting Eq. (8) into (5), we get the following forward recursive relation u_n and backward recursive relation u_{n-1} to find the wave function.

$$u_n = \frac{2\left[1 - \frac{5h^2}{12} k_{n-1}\right] u_{n-1} - \left[1 + \frac{h^2}{12} k_{n-2}\right] u_{n-2}}{\left[1 + \frac{h^2}{12} k_n\right]} \tag{9}$$

$$u_{n-1} = \frac{2\left[1 - \frac{5h^2}{12} k_n\right] u_n - \left[1 + \frac{h^2}{12} k_{n+1}\right] u_{n+1}}{\left[1 + \frac{h^2}{12} k_{n-1}\right]} \tag{10}$$

To find the wave function by using these forward-backward technique, it is necessary to give two initial values for each direction and the first derivative wave function is

$$u'_n = \frac{1}{2h}\left[\left(1 + \frac{h^2}{6} k_{n+1}\right) u_{n+1} - \left(1 + \frac{h^2}{6} k_{n-1}\right) u_{n-1}\right] \tag{11}$$

Since both outward and inward wave functions $u_{out}(r)$ and $u_{in}(r)$ satisfy homogeneous equation, their normalization can always be chosen so that they are set to be equal at the match point r_c. At that point the eigen functions must satisfy the following continuity conditions

$$(u_{out})_{r_c} = (u_{in})_{r_c}, \; (u'_{out})_{r_c} = (u'_{in})_{r_c} \tag{12}$$

A function $G(E)$ can be defined at r_c point whose zeros correspond to the energy eigenvalues as

$$G(E) = \left[\frac{u'_{out}}{u_{out}}\right]_{r_c} - \left[\frac{u'_{in}}{u_{in}}\right]_{r_c} \tag{13}$$

Now we proceed numerically in the following way: firstly, we set a trial energy as an input at $r = 0$ and this energy is increased by the formula $E_n = E + \Delta E$ where ΔE is energy step within the N points. Then the eigen functions of u_{out} and u_{in} for each E_n can be calculated at r_c point and build the $G(E)$ function. In this function, we carefully looked for and checked a change of sign and then perform a fine tuning closing the energy range until the required tolerance. If the value of this function is zero or close to zero, the correct energy eigen value and corresponding eigen function can be obtained simultaneously.

Normalized Wave Function

In order to investigate the properties of nucleon single-particle states, the two wave functions must be taken in normalization condition. The eigen functions of $u_{out}(r)$ and $u_{in}(r)$ obtained from the recursive formulas can be written as

$$u_{out}(r) = A\,\Phi(r), \quad u_{in}(r) = B\,I(r) \tag{14}$$

where A and B are constants and their derivatives also become

$$u'_{out}(r) = A\,\Phi'(r), \quad u'_{in}(r) = B\,I'(r) \tag{15}$$

By substituting Eq. (14) and (15) in Eq. (12), we get

$$(A\Phi)_{r_c} = (B\,I)_{r_c} \text{ and } (A\Phi')_{r_c} = (B\,I')_{r_c} \tag{16}$$

and taking the difference of above equations, we obtain $A=\left[\frac{I-I'}{\Phi-\Phi'}\right]_{r_c}$ $B \equiv f_c B$, where f_c is a scaling factor and this equation relates between constant A and B. We have already got outwards wave function (Φ) and inward wave function (I) from the recursive formulas. After taking their derivative, we can find the constant value A. After obtaining the value of constant A , the value of constant B can be acquired. So Eq. (15) can be represented as

$$u_{out}(r) = f_c\, B\, \Phi(r), \qquad u_{in}(r) = B\, I(r) \tag{17}$$

where B is a global factor and it must be taken into account in the normalization process. Then the normalized constant B can be obtained by using the following normalization conditions

$$\int_0^{r_{\max}} |u_l(r)|^2\, dr = \int_{r_0}^{r_c} |u_{out}(r)|^2 dr + \int_{r_c}^{r_{\max}} |u_{in}(r)|^2\, dr = 1 \tag{18}$$

The global factor $B = \frac{1}{\sqrt{N}}$ and where $N = \left[f_c^2 \int_0^{r_c} |\Phi(r)|^2\, dr + \int_{r_c}^{r_{\max}} |I(r)|^2\, dr \right]$

Then the normalized outwards and inwards eigen functions becomes

$u_{out}(r) = \frac{1}{\sqrt{N}}\ f_c\, \Phi(r)$ from $r = 0$ fm to r_c point and $u_{in}(r) = \frac{1}{\sqrt{N}}\ I(r)$ from $r = r_c$ fm to r_N point.

Interaction

I. Woods-Saxon potential

The Woods-Saxon potential is the sum of a spin-independent central potential, a spin-orbit potential and the Coulomb potential:

$$V(r) = V_o(r) + V_{so}(r)\vec{l}\cdot\vec{s} + V_c(r) \tag{19}$$

$$V_0(r) = \frac{V_0}{1 + \exp\left(\frac{r-R}{a}\right)},\ R = r_0 A^{1/3} \tag{20}$$

where $V_0(r)$ = spin independent central potential, R = nuclear radius,

$$V_{so}(r) = V_{so}\frac{1}{r}\frac{d}{dr}\frac{1}{1+\exp\left(\frac{r-R}{a}\right)} = -V_{so}\frac{1}{ra}\frac{\exp\left(\frac{r-R}{a}\right)}{\left(1+\exp\left(\frac{r-R}{a}\right)\right)^2} \tag{21}$$

$V_{so}(r)$ = spin-orbit potential

$$V_c(r) = \frac{Ze^2}{r} \qquad \text{for } r \geq R \tag{22}$$

$$V_c(r) = \frac{Ze^2}{r}\left[\frac{3}{2} - \frac{r^2}{2R^2}\right] \qquad \text{for } r \le R \tag{23}$$

Parameters

$$V_0 = 53 + \frac{N-Z}{A}V_1 \qquad \text{for protons}$$

$$V_0 = 53 - \frac{N-Z}{A}V_1 \qquad \text{for neutrons}$$

$V_1 = -30$ MeV, $V_{so} = 22$ MeV, $r_0 = 1.25$ fm, $a = 0.65$ fm

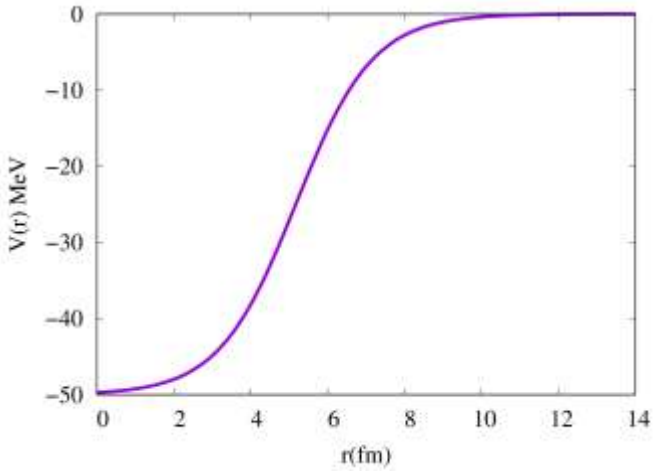


Figure (1) Woods-Saxon potential with spin-orbit for ^{90}Zr

II. Derivation of Spin-orbit Interaction

Woods-Saxon central potential does not have any energy level splitting and so spin-orbit interaction is used to get energy level splitting. Woods-Saxon potential with spin-orbit coupling term is represented as follows.

$$V_{l.s}(r) = V_{so}\left[\frac{\mathrm{h}}{m_\pi c}\right]^2 \left[\vec{l}.\vec{s}\right]\frac{1}{r}\frac{d\rho(r)}{dr} \tag{24}$$

$\rho(r)$ = nuclear density, $\qquad \rho(r) = \dfrac{1}{1+e^{\frac{r-R}{a}}}$ (25)

$$\frac{d\rho(r)}{dr} = \frac{d}{dr}\left[\frac{1}{1+e^{\frac{r-R}{a}}}\right] = \frac{d}{dr}\left[1+e^{\frac{r-R}{a}}\right]^{-1}$$

$$\frac{d\rho(r)}{dr} = -\frac{e^{\frac{r-R}{a}}}{\left[1+e^{\frac{r-R}{a}}\right]^2}\frac{1}{a} \tag{26}$$

The spin-orbit term with the scalar product of the orbital angular momentum operator L and the intrinsic operator S, can be represented by using the total angular momentum.

$$\vec{J} = \vec{L} + \vec{S} \tag{27}$$

$$J^2 = \left(\vec{L} + \vec{S}\right) \cdot \left(\vec{L} + \vec{S}\right) \tag{28}$$

$$J^2 = L^2 + 2\vec{L} \cdot \vec{S} + S^2 \tag{29}$$

The magnitude of the total angular momentum, the orbital angular momentum and the spin angular momentum are

$$J^2 = j(j+1)\mathrm{h}^2, \quad L^2 = \mathrm{l}(\mathrm{l}+1)\mathrm{h}^2, \quad S^2 = s(s+1)\mathrm{h}^2$$

$$J^2 - L^2 - S^2 = 2\vec{L} \cdot \vec{S}$$

$$\vec{L}.\vec{S} = \frac{1}{2}\left[J^2 - L^2 - S^2\right] = \frac{1}{2}\left[j(j+1) - \mathrm{l}(\mathrm{l}+1) - s(s+1)\right]\mathrm{h}^2$$

$$\vec{L}.\vec{S} = \frac{1}{2}\left[j(j+1) - \mathrm{l}(\mathrm{l}+1) - \frac{1}{2}\left(\frac{1}{2}+1\right)\right]\mathrm{h}^2$$

$$\vec{L}.\vec{S} = \frac{1}{2}\left[j(j+1) - \mathrm{l}(\mathrm{l}+1) - \frac{3}{4}\right]\mathrm{h}^2 \tag{30}$$

If $j = \mathrm{l} + \frac{1}{2}$, Eq. (30) becomes $\vec{L}.\vec{S} = \frac{1}{2}\left[\left(\mathrm{l}+\frac{1}{2}\right)\left(\mathrm{l}+\frac{1}{2}+1\right) - \mathrm{l}(\mathrm{l}+1) - \frac{3}{4}\right]\mathrm{h}^2$

$$\vec{L}.\vec{S} = \frac{1}{2}\mathrm{l}\,\mathrm{h}^2 \tag{31}$$

If $j = \mathrm{l} - \frac{1}{2}$, Eq. (30) becomes $\vec{L}.\vec{S} = \frac{1}{2}\left[\left(\mathrm{l}-\frac{1}{2}\right)\left(\mathrm{l}-\frac{1}{2}+1\right) - \mathrm{l}(\mathrm{l}+1) - \frac{3}{4}\right]\mathrm{h}^2$

$$\vec{L}.\vec{S} = -\frac{1}{2}(\mathrm{l}+1)\mathrm{h}^2 \tag{32}$$

There are two possible conditions such as $j = \mathrm{l} + \frac{1}{2}$ and $j = \mathrm{l} - \frac{1}{2}$.

If $j = \mathrm{l} + \frac{1}{2}$, Eq. (24) becomes

$$V_{\mathrm{l}.s}(r) = V_{so}\left[\frac{\mathrm{h}}{m_\pi c}\right]^2 \left(\frac{1}{2}\mathrm{l}\right)\frac{1}{r}\frac{d\rho(r)}{dr} \tag{33}$$

If $j = \mathrm{l} - \frac{1}{2}$, Eq. (24) becomes

$$V_{l.s}(r) = V_{so}\left[\frac{\hbar}{m_\pi c}\right]^2\left(-\frac{1}{2}(l+1)\right)\frac{1}{r}\frac{d\rho(r)}{dr} \tag{34}$$

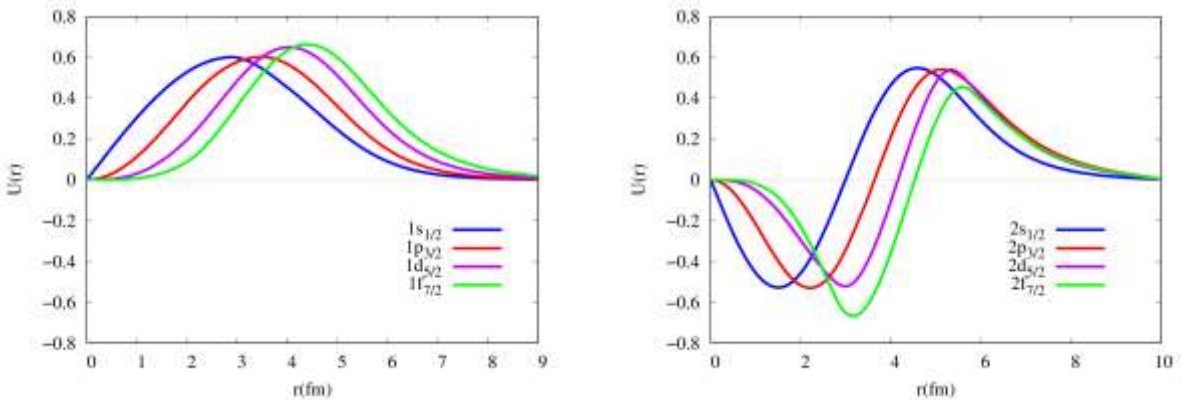
The spin orbit interaction term of Eq. (33) and (34) are substituted in Eq. (19) then we get

$$V(r) = V_0(r) + V_{so}\left[\frac{\hbar}{m_\pi c}\right]^2\left(\frac{1}{2}l\right)\frac{1}{r}\frac{d\rho}{dr} + V_c(r)$$

$$V(r) = V_0(r) + V_{so}\left[\frac{\hbar}{m_\pi c}\right]^2\left(-\frac{1}{2}(l+1)\right)\frac{1}{r}\frac{d\rho}{dr} + V_c(r)$$

Results and Discussions

Firstly, the proton single-particle energies of ^{90}Zr for various states such as s, p, d and f states of $l+\frac{1}{2}$ case and $l-\frac{1}{2}$ case were calculated by using phenomenological Woods-Saxon potential and the calculated results are shown in Fig. (2) and (3).



(a) (b)

Figure (2) (a) Proton wave functions $\left(l+\frac{1}{2}\right)$ case for $1s_{1/2}, 1p_{3/2}, 1d_{5/2}, 1f_{7/2}$ states

(b) Proton wave functions $\left(l+\frac{1}{2}\right)$ case for $2s_{1/2}, 2p_{3/2}, 2d_{5/2}, 2f_{7/2}$ states

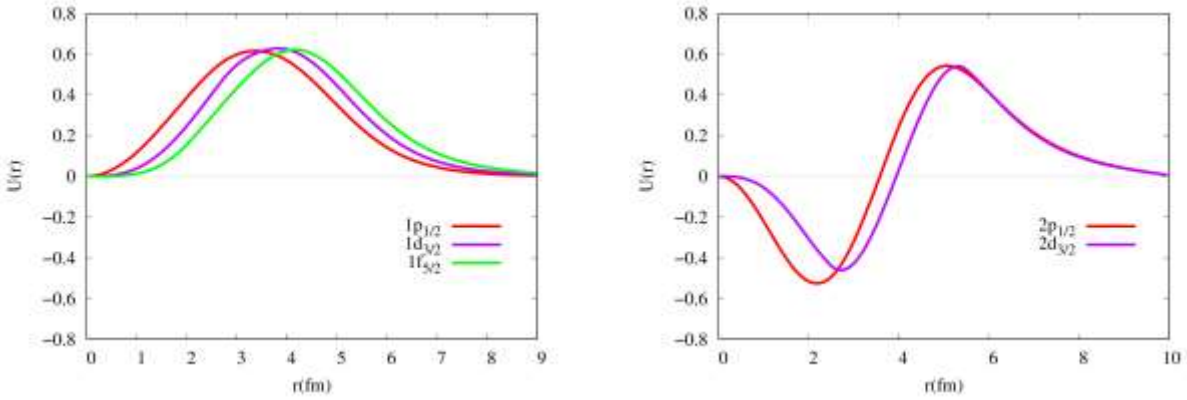


Figure (3) (a) Proton wave functions $\left(l-\frac{1}{2}\right)$ case for $1p_{1/2}, 1d_{3/2}, 1f_{5/2}$ states

(b) Proton wave functions $\left(l-\frac{1}{2}\right)$ case for $2p_{1/2}, 2d_{3/2}$ states

Fig. (2) and (3) show the calculated results of various s states, p states and d states proton wave functions with phenomenological Woods-Saxon potential for ^{90}Zr . The wave functions are shifted to outer region for higher orbital angular momentum and it is seen that all wave functions are finite. There is no node in 1s, 1p, 1d and 1f states and one node in 2s, 2p, 2d and 2f states of both $\left(l + \frac{1}{2}\right)$ and $\left(l - \frac{1}{2}\right)$ cases. Similarly, the neutron single-particle energies of ^{90}Zr in various states were obtained in the same way. But neutron is a chargeless particle so Coulomb potential are not taken into account in this calculation. Then the calculated results are shown in Figure (4) and (5).

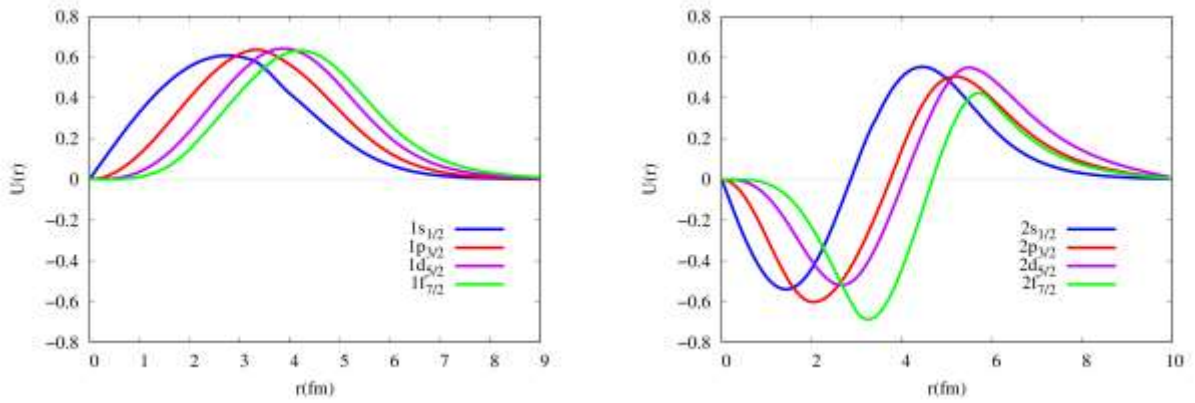


Figure (4) (a) Neutron wave functions $\left(l + \frac{1}{2}\right)$ case for $1s_{1/2}, 1p_{3/2}, 1d_{5/2}, 1f_{7/2}$ states

(b) Neutron wave functions $\left(l + \frac{1}{2}\right)$ case for $2s_{1/2}, 2p_{3/2}, 2d_{5/2}, 2f_{7/2}$ states

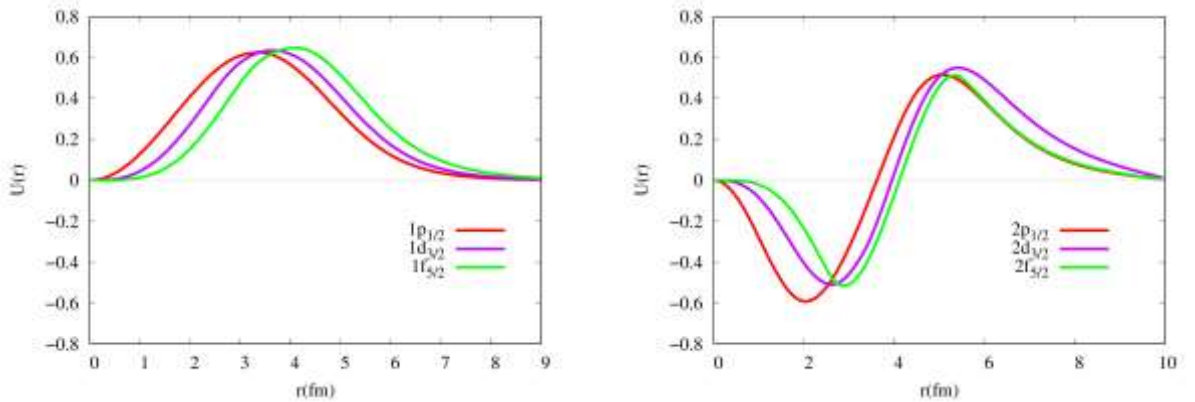
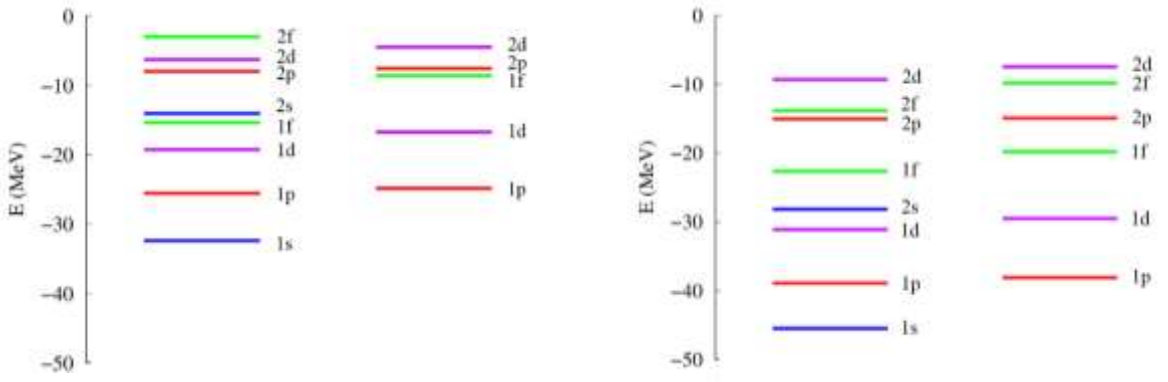


Figure (5) (a) Neutron wave functions $\left(l - \frac{1}{2}\right)$ case for $1p_{1/2}, 1d_{3/2}, 1f_{5/2}$ states

(b) Neutron wave functions $\left(l - \frac{1}{2}\right)$ case for $2p_{1/2}, 2d_{3/2}, 2f_{5/2}$ states

Figure (6) (a) and (b) shows energy levels for proton and neutron state for $\left(l + \frac{1}{2}\right)$ and $\left(l - \frac{1}{2}\right)$ cases. According to this figure, 1s state has the largest binding energy among the other states. If the nucleon is in the innermost shell of the nucleus, it will have largest binding energy and gradually decreases with shell level ordering.

Finally, the calculated results were compared with two sets parameters of Skyrme type effective nucleon-nucleon interaction BsK1, SVIII and the available experimental data in Table (1) and (2). The results were agreed with these two theoretical and experimental results.



(a) (b)

Figure (6) (a) Proton single-particle energy levels for $\left(l+\frac{1}{2}\right)$ case and $\left(l-\frac{1}{2}\right)$ case

(b) Neutron single-particle energy levels for $\left(l+\frac{1}{2}\right)$ case and $\left(l-\frac{1}{2}\right)$ case

Table 1 Comparison of experimental results, Skyrme type interaction based two set parameters and our calculated results for proton single-particle energies in ^{90}Zr

Subshell	**Exp**	**Skyrme type effective nucleon-nucleon interaction**		**Our calculated results**
		BsK1	**SVIII**	
$1s_{1/2}$	43±8	33.02	32.44	32.36
$2s_{1/2}$	-	16.78	16.58	15.84
$1p_{3/2}$	35±8	27.17	27.72	25.51
$2p_{3/2}$	-	8.79	8.02	7.92
$1d_{5/2}$	27±8	21.27	21.72	19.21
$2d_{5/2}$	-	-	-	7.22
$1f_{7/2}$	-	14.47	14.70	15.32
$2f_{7/2}$	-	-	-	2.93
$1p_{1/2}$	33±8	24.45	26.29	24.80
$2p_{1/2}$	-	7.21	6.58	8.30
$1d_{3/2}$	26±8	17.63	18.66	16.69
$2d_{3/2}$	-	-	-	4.43
$1f_{5/2}$	-	8.65	9.65	8.53

Table 2 Comparison of experimental results, Skyrme type interaction based two set parameters and our calculated results for neutron single-particle energies in ^{90}Zr

Subshell	Exp	Skyrme type effective nucleon-nucleon interaction		Our calculated results
		BsK1	SVIII	
$1s_{1/2}$	-	45.31	43.78	45.51
$2s_{1/2}$	-	27.85	27.54	28.14
$1p_{3/2}$	-	39.19	37.94	38.90
$2p_{3/2}$	15.10	15.78	15.17	15.01
$1d_{5/2}$	-	30.37	30.27	31.17
$2d_{5/2}$	-	8.71	8.74	9.30
$1f_{7/2}$	-	22.00	21.95	22.62
$2f_{7/2}$	-	-	-	13.81
$1p_{1/2}$	-	38.27	37.81	38.13
$2p_{1/2}$	13.60	14.87	14.52	14.91
$1d_{3/2}$	-	28.98	28.48	29.5
$2d_{3/2}$	-	7.11	7.40	7.42
$1f_{5/2}$	18.50	19.19	18.98	19.81
$2f_{5/2}$	-	-	-	9.83

Conclusion

In this paper, the nucleon wave functions and their single-particle energy levels in ^{90}Zr were investigated by solving one-body Schrödinger equation within the frame work of numerov method. The results of all of wave functions were found to be convergent. In this investigation, phenomenological Woods-Saxon central potential including spin-orbit interaction was used. The numerical calculation was solved by using FORTRAN-90 code. Then the calculated results were compared with two set parameters of Skyrme type based nucleon-nucleon interaction and available experimental results. As a result, the calculated shell structures of nucleon single-particle energies were agreed with both theoretical and experimental results. Therefore, numerov method is reliable for investigation of single-particle energy of nuclei and our program code is also reliable to use one body potential form.

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