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Bound-state energy of double magic number plus one nucleon nuclei with relativistic mean-field approach

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Abstract. In this work, we have obtained energy levels and charge radius for the β-stability line nucleus, in relativistic shell model. In this model, we considered a close shell for each nucleus containing double magic number and a single nucleon energy level. Here we have taken ^{41}Ca with a single neutron in the ^{40}Ca core as an illustrative example. Then we have selected the Eckart plus Hulthen potentials for interaction between the core and the single nucleon. By using parametric Nikiforov–Uvarov (PNU) method, we have calculated the energy values and wave function. Finally, we have calculated the charge radius for ^{17}O, ^{41}Ca, ^{49}Ca and ^{57}Ni. Our results are in agreement with experimental values and hence this model can be applied for similar nuclei.

Keywords. Shell model; Dirac equation; Eckart potential; Hulthen potential; parametric Nikiforov–Uvarov method.

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1. Introduction

Some static properties of the nucleus, such as energy levels and charge radius, are useful for describing the structure of the nucleus. The nuclear charge radius plays a key role in studying the characteristics of the nucleus and testing theoretical models of the nuclei as well as in studying astrophysics and atomic physics. The calcium isotopes have received much attention due to its rich experimental results in binding energy, density distribution, single-particle energy, radius, etc. It is useful to calculate these quantities to test microscopic theory by future experiments [1]. The study of nuclei under extreme conditions has always been a necessity to understand the nuclear forces. As early as 1934, Elsasser [2] noticed the existence of special numbers of neutrons and protons which confer a particularly stable configuration to the corresponding nuclei. In analogy with atomic electrons, he correlated these numbers with closed shells in a model of non-interacting nucleons occupying energy levels generated by a potential well. More than a decade later, the study of shell structure regained interest through the review of M Goeppert-Mayer which has a large quantity of precise experimental data, which were pointers to the existence of closed shells at numbers 8, 20, 50, 82 and 126 [3]. Understanding the evolution of shell structure from the valley of stability to neutron-rich extremes represents a key challenge in nuclear structure. With a closed proton shell, the ^{17}O, ^{41}Ca, ^{49}Ca and ^{57}Ni isotopes provide an ideal region to investigate shell formation and evolution in medium mass nuclei from nuclear forces [4,5]. We consider ^{17}O, ^{41}Ca, ^{49}Ca and ^{57}Ni isotopes. As these isotopes have double magic number with a single neutron on top of the close core, these isotopes are in the region of the β-stability line nucleus.

The first step of the shell model to study the energy levels of nuclei is to consider the nucleon–nucleon potentials, which reproduce the nucleon–nucleon scattering data and the properties of the nuclei [6,7]. There are many nucleon–nucleon potentials such as Kratzer potential [8,9], Woods–Saxon potential [10,11], Scarf potential [12], Hartmann potential [13,14], Rosen Morse potential [15,16], Hulthen potential [17] and Eckart potential [18,19] that reproduce these data. The Eckart potential which has been studied by many researchers is one of the most important exponential-type potential in physics and chemical physics [20,21].

In this work, we use shell model to calculate the energy levels and charge radius for ^{17}O, ^{41}Ca, ^{49}Ca and ^{57}Ni isotopes. We consider ^{41}Ca as a single neutron and ^{40}Ca core. As these isotopes have one neutron out of the core, we utilize the relativistic Dirac equation to investigate them. These isotopes can be considered as a single particle. We apply the modified Eckart plus Hulthen potentials between the core and a single particle because these potentials are important nuclear potentials for describing the interaction between the single nucleon and the whole nuclei. Now that the *NN* potential is selected, the next step is to solve the Dirac equation for the nuclei under investigation. Several numerical and analytical methods have been used to solve the problem of the Dirac equation by using realistic nuclear potentials. Some of these methods are: the CRCGV [21], the NCSM [22], the EIHH [23], supersymmetric quantum mechanics [24–26], asymptotic iteration method (AIM) [27,28], factorization method [29,30], Laplace transform approach [31], GPS method [32,33], the path integral method [34–36] and the Nikiforov–Uvarov (NU) method [37–39]. We use the parametric Nikiforov–Uvarov (PNU) method to solve the Dirac equation.

The organization of this paper is as follows: in §2, the PNU method is reviewed. In §3 energy spectrum for the isotopes is presented. Conclusion is given in §4.

2. Review of parametric Nikiforov–Uvarov method

The parametric form of the NU method takes the form [37–39]

$$\left[\frac{d^2}{ds^2}+\frac{c_1-c_2s}{s(1-c_3s)}\frac{d}{ds}+\frac{(-p_2s^2+p_1s-p_0)}{s^2(1-c_3s)^2}\right]\Psi_n(s)=0. \quad (1)$$

The energy equation and wave function respectively are obtained from

$$nc_2-(2n+1)c_5+(2n+1)(\sqrt{c_9}+c_3\sqrt{c_8}) +n(n-1)c_3+c_7+2c_3c_8+2\sqrt{c_8c_9}=0, \quad (2)$$

$$\Psi_{n,k}(s)=N_{n,k}s^{c_{12}}(1-c_3s)^{c_{13}}P_n^{(c_{10},c_{11})}(1-2c_3s), \quad (3)$$

where

$$c_4=\frac{1}{2}(1-c_1),\quad c_5=\frac{1}{2}(c_2-2c_3),$$
$$c_6=c_5^2+p_2,\quad c_7=2c_4c_5-p_1,$$
$$c_8=c_4^2+p_0,\quad c_9=c_3(c_7+c_3c_8)+c_6,$$
$$c_{10}=c_1+2c_4+2\sqrt{c_8}-1>-1,$$
$$c_{11}=1-c_1-2c_4+\frac{2}{c_3}\sqrt{c_9}>-1,\quad c_3\neq 0,$$
$$c_{12}=c_4+\sqrt{c_8}>0,$$
$$c_{13}=-c_4+\frac{1}{c_3}(\sqrt{c_9}-c_5)>0,\quad c_3\neq 0. \quad (4)$$

The values of the coefficients c_i ($i = 4, 5,\ldots,13$) depend on p_i ($i = 0, 1, 2$) and p_i depend on energy so the energy levels depended on the coefficients c_i and we could obtain the energy levels by solving eq. (2) numerically.

3. Energy spectrum for the isotopes

The wave function for the Dirac equation can be calculated as

$$\Psi_{n_r,k}(r,\theta,\phi)=\frac{1}{r}\begin{bmatrix}F_{n_r,k}(r)Y_{jm}^{l}(\theta,\phi)\\ iG_{n_r,k}(r)Y_{jm}^{\tilde{l}}(\theta,\phi)\end{bmatrix}, \quad (5)$$

where $F_{n_r,k}(r)$ and $G_{n_r,k}(r)$ are upper and lower components, $Y_{jm}^{l}(\theta,\phi)$ and $Y_{jm}^{\tilde{l}}(\theta,\phi)$ are the spherical harmonic functions. n_r is the radial quantum number and m is the projection of the angular momentum on the z-axis. The orbital angular momentum quantum numbers l and l' represent the spin and pseudospin quantum numbers.

Under the condition of spin symmetry, i.e. $\Delta(r) = 0$, the upper component Dirac equation can be written as [40]

$$\left(-\frac{d^2}{dr^2}+\frac{k(k+1)}{r^2}+\frac{1}{\hbar^2c^2}[Mc^2+E] \times\left[Mc^2-E+\sum(r)\right]\right)F_{n_r,k}(r)=0. \quad (6)$$

The modified Eckart plus Hulthen potential is defined as [17–19]

$$V(r)=v_0\mathrm{cosech}^2(\alpha r)+v_1\frac{e^{-2\alpha r}}{(1-e^{-2\alpha r})}, \quad (7)$$

where the parameters v_0 and v_1 are real parameters, which are strength parameters, and the parameter α is related to the range of the potential.

Under the condition of spin symmetry, sum of the potentials $V(r)$ and $S(r)$ can be written as

$$\sum(r)=8v_0\frac{e^{-2\alpha r}}{(1-e^{-2\alpha r})^2}+2v_1\frac{e^{-2\alpha r}}{(1-e^{-2\alpha r})}. \quad (8)$$

Substituting the transformation $s = \exp(-2\alpha r)$ into eq. (5), we find

$$F''(s) + \frac{1}{s}F'(s) + \frac{1}{4\alpha s^2}\left\{\frac{(E^2 - M^2c^4)}{\hbar^2c^2} - \frac{(E + Mc^2)}{\hbar^2c^2} \times \left[8v_0\frac{s}{(1-s)^2} + 2v_1\frac{s}{(1-s)}\right] - 4\alpha^2\frac{k(k+1)}{(1-s)^2}\right\}F(s) = 0. \quad (9)$$

Equation (9) is exactly solvable only for $k = 0$. In order to obtain the analytical solutions of eq. (9), we employ the improved Pekeris approximation and replace the spin–orbit coupling term with the expression that is valid for $\alpha \leq 1$ [41,42].

$$\frac{k(k+1)}{r^2} \approx \frac{4\alpha^2 k(k+1)}{(\mathrm{e}^{-2\alpha r} - 1)^2}. \quad (10)$$

We can write eq. (9) as given below:

$$F''_{n,k}(s) + \frac{(1-s)}{s(1-s)}F'_{n,k}(s) + \frac{1}{s^2(1-s)^2} \times [-p_2s^2 + p_1s - p_0]F_{n,k}(s) = 0, \quad (11)$$

where the parameters p_2, p_1 and p_0 are as follows:

$$p_2 = -\frac{(E + Mc^2)}{4\alpha^2\hbar^2c^2}[2v_1 + (E - Mc^2)],$$
$$p_1 = -\frac{(E + Mc^2)}{4\alpha^2\hbar^2c^2}[8v_0 + 2v_1 + 2(E - Mc^2)],$$
$$p_0 = k(k+1) - \frac{(E^2 - M^2c^4)}{4\alpha^2\hbar^2c^2}. \quad (12)$$

Now comparing eq. (11) with eq. (1), we obtain the coefficients c_i ($i = 1, 2, 3$) as follows:

$$c_1 = c_2 = c_3 = 1. \quad (13)$$

The values of the coefficients c_i ($i = 4, 5, \ldots, 13$) are also found from eq. (4) as below:

$$c_4 = 0, \quad c_5 = -\frac{1}{2},$$
$$c_6 = \frac{1}{4} + p_2, \quad c_7 = -p_1,$$
$$c_8 = p_0, \quad c_9 = p_2 - p_1 + p_0 + \frac{1}{4},$$
$$c_{10} = 2\sqrt{p_0}, \quad c_{11} = 2\sqrt{p_2 - p_1 + p_0 + \frac{1}{4}},$$
$$c_{12} = \sqrt{p_0}, \quad c_{13} = \frac{1}{2} + \sqrt{p_2 - p_1 + p_0 + \frac{1}{4}}. \quad (14)$$

With respect to eq. (2) in the PNU method, we attain the energy relation as

$$2\sqrt{p_0\left(p_2 - p_1 + p_0 + \frac{1}{4}\right)} + (2n+1)\sqrt{p_2 - p_1 + p_0 + \frac{1}{4}} + (2n+1)\sqrt{p_0} + 2p_0 - p_1 + \left(n + \frac{1}{2}\right)^2 + \frac{1}{4} = 0. \quad (15)$$

The ground-state and first excited energies of ^{17}O, ^{41}Ca, ^{49}Ca and ^{57}Ni isotopes are obtained by using eq. (15). These results are compared with the experimental data in table 1 [44]. The calculated energy levels are in good agreement with experimental values. Therefore, the proposed model can well be used to investigate other similar isotopes. With respect to eq. (3) in PNU method [39,43,45] and eq. (14), the upper component of the Dirac spinor is given by eq. (16).

$$F_{n_r,k}(r) = N(\mathrm{e}^{-2\alpha r})^{\sqrt{p_0}} \times (1 - \mathrm{e}^{-2\alpha r})^{\sqrt{p_2 - p_1 + p_0 + \frac{1}{4}} + \frac{1}{2}} \times P_n^{2\sqrt{p_0}, 2\sqrt{p_2 - p_1 + p_0 + \frac{1}{4}}}(1 - 2\mathrm{e}^{-2\alpha r}), \quad (16)$$

where N is the normalization constant. The lower component of the Dirac spinor can be calculated from eq. (16) as

$$G_{n_r,k}(r) = \frac{\hbar^2c^2}{E + Mc^2}\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r}\right)F_{n_r,k}(r). \quad (17)$$

The wave function can be calculated by substituting eqs (16) and (17) in eq. (5) as

$$\psi_{n_r,k}(r,\theta,\phi) = N\begin{bmatrix} Y^l_{jm}(\theta,\phi) \\ \frac{i}{[M + E_{n_r,k}]}\left[\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r}\right]Y^{\tilde{l}}_{jm}(\theta,\phi)\end{bmatrix} \times \frac{(\mathrm{e}^{-2\alpha r})^{\sqrt{p_0}}}{r}(1 - \mathrm{e}^{-2\alpha r})^{\sqrt{p_2 - p_1 + p_0 + \frac{1}{4}} + \frac{1}{2}} \times P_n^{2\sqrt{p_0}, 2\sqrt{p_2 - p_1 + p_0 + \frac{1}{4}}}(1 - 2\mathrm{e}^{-2\alpha r}). \quad (18)$$

We calculate the charge radius by using eqs (18) and (19) for ^{17}O, ^{41}Ca, ^{49}Ca and ^{57}Ni isotopes.

$$\langle r^2\rangle^{1/2} = \left(\frac{\int \psi^*_{n_r,k}(r)r^2\psi_{n_r,k}(r)\mathrm{d}^3r}{\int \psi^*_{n_r,k}(r)\psi_{n_r,k}(r)\mathrm{d}^3r}\right)^{1/2}. \quad (19)$$

Table 1. The ground-state and the first excited energy (MeV) for the isotopes.

Isotope	State	Our work	Exp.
^{17}O	$E_{1d5/2}$	−131.7245	−131.7624 [44]
	$E_{2s1/2}$	−130.8210	−130.8916 [44]
^{41}Ca	$E_{1f7/2}$	−350.4029	−350.4148 [44]
	$E_{2p3/2}$	−348.4377	−348.4748 [44]
^{49}Ca	$E_{2p3/2}$	−421.1041	−421.1475 [44]
	$E_{1f5/2}$	−417.5306	−417.5625 [44]
^{57}Ni	$E_{2p3/2}$	−494.1924	−494.2413 [44]
	$E_{1f5/2}$	−493.4282	−493.4728 [44]

Table 2. The charge radius (fm) for ground-state isotopes.

Isotope	$\langle r^2\rangle^{1/2}_{\text{our work}}$(fm)	$\langle r^2\rangle^{1/2}_{\text{Exp}}$ (fm)
^{17}O	2.6616	2.6953 [46]
^{41}Ca	3.4688	3.4780 [46]
^{49}Ca	3.4822	–
^{57}Ni	3.7352	–

In table 2 we show the calculated charge radii for the ground-state isotopes, and compared them with the experimental data. For example, the calculated parameters of the modified potential are: α (fm^{-1}) $= 0.0127$, $V_0 = 0.1292$, $V_1 = -67.929$. The obtained charge radii for the ground-state isotopes are in good agreement with the experimental value. The results show that our model can be used to investigate other similar isotopes, because Dirac equation specially gives good result for single-particle systems. Dirac equation describes particles of half-integer spin. So this model cannot consider nuclei with integer spin.

4. Conclusions

In this paper, we have calculated some energy levels of ^{17}O, ^{41}Ca, ^{49}Ca and ^{57}Ni isotopes with modified Eckart plus Hulthen potentials using the PNU method. We obtained the energy levels and wave functions for these isotopes. The wave functions satisfy the boundary conditions; also we obtained the charge radii and compared them with experimental values. The results are in agreement with experimental values and hence contain important physics.

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