Consideration of some static properties for doubly-magic nuclei of ^{41}Ca and ^{17}O in relativistic systems

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We have considered some static properties of the ^{41}Ca and ^{17}O in the relativistic shell model. The nuclei ^{41}Ca and ^{17}O can be modeled as a doubly-magic ^{40}Ca and ^{16}O core, with one additional nucleon (valence) in the lf$_{7/2}$ and 1d$_{5/2}$ levels. Then we have selected the modified Hulthen plus quadratic Yukawa potentials for interaction between core and single nucleon. By using Parametric Nikiforov-Uvarov method, we have calculated the energy values and wave function. Finally, we calculated the charge radius and electric quadruple moment for ^{41}Ca and ^{17}O. Our results were in agreement with experimental values and hence this model could be applied for similar nuclei.

1. Introduction

The goals of the study of nuclear physics are to understand the force between nucleons, the structure of nuclei, and the nature of nuclear interactions with each other and with other subatomic particles. Nuclear structure research focuses on properties of nuclei such as the energies of excited states, nuclear shapes, electromagnetic moments and transition rates between excited states and the ground state, and how nuclei transform into different nuclei.

In addition to providing information about the structure of individual nuclei, nuclear structure studies provide experimental information that can be used by theorists to explain the nature of nuclear forces [1]. The best evidence for single-particle behavior is found near magic (also called closed-shell) nuclei, where the number of protons and/or neutrons in a nucleus fills the last shell before a major or minor shell gap. For example, the nuclei ^{41}Ca and ^{17}O can be modeled as a doubly-magic ^{40}Ca and ^{16}O core, with one additional (valence) nucleon in the lf$_{7/2}$ and 1d$_{5/2}$ levels. The ground-state spin and parity of ^{41}Ca and ^{17}O are $J^{\pi}=7/2^{-}$, $5/2^{+}$ which corresponds to the spin and parity of the level where the valence nucleon resides [2].

The standard analytical method to solve the Schrödinger equation, Dirac equation, and Klein-Gordon equation with a variable coefficient is to expand the solution in a power series of the independent variable r and then find the recursion relations for all the expansion coefficients [20]. This method has more details to reach the solution. Numerical and analytical methods complement each other to find an exact or approximate solution of the quantum, and each would be poorer without the other.

The ab-initio method is one of the numerical methods that have been used to explore the structure of light nuclei. Recently, Pieper and Wiringa used ab-initio calculations based on the Green's function Monte Carlo (GFMC) method for the ^{4}He ground state energy and radius obtained from the nucleon-nucleon (NN) Argonne V_8 potential [21, 22]. But in our article we use simple "hand-power methods", namely analytical methods, because it's more revealing to see the solution stages of the problem, and so it would be more meaningful than the numerical solution.

Since these isotopes have one nucleon out of core, we utilize the relativistic Dirac equation to investigate them. We apply the modified Hulthen plus quadratic Yukawa potentials between core and a single particle because these potentials are important nuclear potentials for description of interaction between single nucleon and whole nuclei. Now that the potential is selected, the next step is solution of the Dirac equation for the nuclei under investigation. We use the Parametric Nikiforov-Uvarov (PNU) method [3, 4, 5] to solve the Dirac equation.

The organization of this paper is as follows: in Sec. 2, the PNU method is reviewed; in Sec. 3 we review Basic Dirac Equations briefly; in Sec. 4 Relativistic Analytical Method is presented, and Results and discussion are given in Sec. 5.

2. Review of Parametric Nikiforov-Uvarov Method

The NU method has been used to solve the Schrodinger, Dirac, and Klein-Gordon wave equations for a certain kind of potential. In this method the differential equations can be written as follows [4, 6].

$$\Psi''(s)+\frac{\tilde{\tau}(s)}{\sigma(s)}\Psi'(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\Psi(s)=0 \quad (1)$$

Where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most second degree and $\tilde{\tau}(s)$ is a first degree polynomials.

Schrodinger-like equation (Eqn. (1)) in a rather more general form as [7, 8]

$$\left[\frac{d^2}{ds^2}+\frac{\varepsilon_1-\varepsilon_2 s}{s(1-\varepsilon_3 s)}\frac{d}{ds}+\frac{(-\chi_2 s^2+\chi_1 s-\chi_0)}{s^2(1-\varepsilon_3 s)^2}\right]\Psi_n(s)=0 \quad (2)$$

We set the wave function as:

$$\Psi(s)=f(s)y(s) \quad (3)$$

Secondly, we compare Eqn. (2) with its counterpart Eq. (1) to obtain the following parameter values,

$$\tilde{\tau}(s)=\varepsilon_1-\varepsilon_2 s \quad \sigma(s)=s(1-\varepsilon_3 s),$$

$$\tilde{\sigma}(s)=-\chi_2 s^2+\chi_1 s-\chi_0 \quad (4)$$

Now, following the NU method, we obtain the following energy equation:

$$n\epsilon_2-(2n+1)\epsilon_5+(2n+1)(\sqrt{\epsilon_9}+\epsilon_3\sqrt{\epsilon_8}+n(n-1)\epsilon_3+\epsilon_7+2\epsilon_3\epsilon_8+2\sqrt{\epsilon_8\epsilon_9}=0 \quad (5)$$

And the corresponding wave functions

$$\rho(s)=s^{\varepsilon_{10}}(1-\varepsilon_3 s)^{\varepsilon_{11}}, \quad \Phi(s)=s^{\varepsilon_{12}}(1-\varepsilon_3 s)^{\varepsilon_{13}}$$

$$\varepsilon_{12}>0,\varepsilon_{13}>0 \quad (6)$$

,

$$y_n(s)=P_n^{(\varepsilon_{10},\varepsilon_{11})}(1-2\varepsilon_3 s),\varepsilon_{10}>-1,\varepsilon_{11}>-1 \quad (7)$$

and

$$\Psi_{n,k}(s)=N_{n,k}s^{\varepsilon_{12}}(1-\varepsilon_3 s)^{\varepsilon_{13}}P_n^{(\varepsilon_{10},\varepsilon_{11})}(1-2\varepsilon_3 s) \quad (8)$$

Where $P_n^{(\mu,v)}(x)$ ($\mu>-1$, $v>-1$ and $x \in [-1, 1]$) are Jacobi polynomials with the following constants:

$$\varepsilon_4=\frac{1}{2}(1-\varepsilon_1) \qquad \varepsilon_5=\frac{1}{2}(\varepsilon_2-2\varepsilon_3)$$

$$\varepsilon_6=\varepsilon_5^2+\chi_2 \qquad \varepsilon_7=2\varepsilon_4\varepsilon_5-\chi_1$$

$$\varepsilon_8=\varepsilon_4^2+\chi_0 \qquad \varepsilon_9=\varepsilon_3(\varepsilon_7+\varepsilon_3\varepsilon_8)+\varepsilon_6$$

$$\varepsilon_{10}=\varepsilon_1+2\varepsilon_4+2\sqrt{\varepsilon_8}-1>-1$$

$$\varepsilon_{11}=1-\varepsilon_1-2\varepsilon_4+\frac{2}{\varepsilon_3}\sqrt{\varepsilon_9}>-1,\varepsilon_3\neq 0$$

$$\varepsilon_{12}=\varepsilon_4+\sqrt{\varepsilon_8}>0$$

$$\varepsilon_{13}=-\varepsilon_4+\frac{1}{\varepsilon_3}\left(\sqrt{\varepsilon_9}-\varepsilon_5\right)>0,\varepsilon_3\neq 0 \quad (9)$$

Where $\varepsilon_{12}>0$, $\varepsilon_{13}>0$ and $s \in [0, 1/\varepsilon_3]$, $\varepsilon_3\neq 0$, In the rather more special case of $\varepsilon_3=0$, ε_{11}, ε_{13} becomes

$$\varepsilon_{11}=\varepsilon_2-2\varepsilon_5+2(\sqrt{\varepsilon_9}+\varepsilon_3\sqrt{\varepsilon_8}$$

$$\varepsilon_{13}=\varepsilon_5-(\sqrt{\varepsilon_9}-\varepsilon_3\sqrt{\varepsilon_8}) \quad (10)$$

The wave function (Eqn.8) becomes

$$\lim_{\varepsilon_3\to 0}P_n^{(\varepsilon_{10},\varepsilon_{11})}(1-2\varepsilon_3 s)=L_n^{\varepsilon_{10}}(\varepsilon_{11}s) \quad (11)$$

$$\lim_{\varepsilon_3\to 0}(1-2\varepsilon_3 s)^{\varepsilon_{12}}=e^{\varepsilon_{13}s} \quad (12)$$

To make the application of the NU method simpler and direct without need to check the validity of solution. We present a shortcut for the method. Hence, firstly, we write the general form of the

$$\Psi_{n,k}(s)=N_{n,k}s^{\varepsilon_{12}}e^{\varepsilon_{13}s}L_n^{\varepsilon_{10}}(\varepsilon_{11}s) \quad (13)$$

And $L_n^{\alpha}(x)$ are the Laguerre polynomials [9].

3. Basic Dirac Equations

In the relativistic description, the Dirac equation of a single-nucleon with the mass moving in an attractive scalar potential S(r) and a repulsive vector potential V (r) can be written as [10]

$$[-i\hbar c\hat{\alpha}.\hat{\nabla}+\hat{\beta}(Mc^2+S(r))]\Psi_{n_r,k}=[E-V(r)]\Psi_{n_r,k} \quad (14)$$

Where E is the relativistic energy, M is the mass of a single particle and α and β are the 4 ×4 Dirac matrices. For a particle in a central field, the total angular momentum J and $\hat{K}=-\hat{\beta}(\hat{\alpha}.\hat{L}+\hbar)$ commute with the Dirac Hamiltonian where L is the orbital angular momentum. For a given total angular momentum j, the Eigen-values of the $\hat{K}$ are k=± (j+1/2) where negative sign is for aligned spin and positive sign is for unaligned spin. The wave-functions can be classified according to their angular momentum *j* and spin-orbit quantum number k as follows:

$$\Psi_{n_r,k}(r,\theta,\phi)=\frac{1}{r}\begin{bmatrix}F_{n_r,k}(r)Y_{jm}^{l}(\theta,\phi)\\ iG_{n_r,k}(r)Y_{jm}^{\tilde{l}}(\theta,\phi)\end{bmatrix} \quad (15)$$

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 $\tilde{l}$ represent to the spin and pseudo-spin quantum numbers. Substituting Eqn. (15) into Eqn. (14), we obtain couple equations for the radial part of the Dirac equation as follows:

$$\begin{cases}(\frac{d}{dr}+\frac{k}{r})F_{n_r,k}(r)=\frac{1}{\hbar c}[Mc^2+E-\Delta(r)]G_{n_r,k}(r)\\ (\frac{d}{dr}-\frac{k}{r})G_{n_r,k}(r)=\frac{1}{\hbar c}[Mc^2-E+\Sigma(r)]F_{n_r,k}(r)\end{cases} \quad (16)$$

Where Δ (r)=V(r)-S(r) and ∑(r)=V(r)+S(r) are the difference and the sum of the potentials V(r) and S(r), respectively.

Under the condition of the spin symmetry, i.e., Δ(r) =0, Eqn. (16) reduces into

$$\left(-\frac{d^2}{dr^2}+\frac{k(k+1)}{r^2}+\frac{1}{\hbar^2c^2}[Mc^2+E][Mc^2-E+\Sigma(r)]\right)F_{n_r,k}(r)=0 \quad (17)$$

Under the condition of the pseudo-spin symmetry, i.e., $\sum(r)=0$ Eqn. (16) turns to the following form

$$\left(-\frac{d^2}{dr^2}+\frac{k(k-1)}{r^2}+\frac{1}{\hbar^2c^2}[Mc^2-E][Mc^2+E-\Delta(r)]\right)G_{n_r,k}(r)=0 \tag{18}$$

We consider bound state solutions that demand the radial components satisfying $F_{n_r,k}(0)=G_{n_r,k}(0)=0$, and $F_{n_r,k}(\infty)=G_{n_r,k}(\infty)=0$ [10].

4. Relativistic Analytical Method

4.1 Energy Spectrum of ^{41}Ca and ^{17}O Isotope

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

$$\left(-\frac{d^2}{dr^2}+\frac{k(k+1)}{r^2}+\frac{1}{\hbar^2c^2}[Mc^2+E][Mc^2-E+\Sigma(r)]\right)F_{n_r,k}(r)=0 \tag{19}$$

The modified Hulthen plus quadratic Yukawa potentials is defined as [11, 12]

$$V(r)=-\frac{v_0e^{-\alpha r}}{\alpha(1-e^{-\alpha r})}+\frac{v_1e^{-\alpha r}}{\alpha r^2} \tag{20}$$

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

Using the transformation, $s=\exp(-\alpha r)$ [11], Eqn. (19) brings into the form

$$F''(s)+\frac{1}{s}F'(s)+\frac{1}{s^2}\left\{\frac{E^2-M^2c^4}{\hbar^2c^2\alpha^2}+\frac{E^2+M^2c^4}{\hbar^2c^2\alpha^2}\left[-2v_0\frac{s}{\alpha(1-s)^2}2v_1\frac{s^2}{\alpha(1-s)^2}\right]-k(k+1)\frac{s}{(1-s)^2}\right\}F(s)=0 \tag{21}$$

Eqn. (21) is exactly solvable only for the case of k = 0. In order to obtain the analytical solutions of Eqn. (21), we employ the improved Pekeris approximation and replace the spin–orbit coupling term with the expression that is valid for $\alpha \le 1$, [13-14].

$$\frac{k(k+1)}{r^2}\approx k(k+1)\frac{\alpha^2e^{-\alpha r}}{(1-e^{-\alpha r})^2} \tag{22}$$

We can write the Eqn. (24) as summarized below

$$F''_{n,k}(s)+\frac{(1-s)}{s(1-s)}F'_{n,k}(s)+\frac{1}{s^2(1-s)^2}[-\chi_2s^2+\chi_1s-\chi_0]F_{n,k}(s)=0 \tag{23}$$

Where the parameters χ_2, χ_1 and χ_0 are considered as follows:

$$\chi_2=2\beta\left(\frac{v_0}{\alpha}+\frac{v_1}{\alpha}\right)-\gamma$$

$$\chi_1=2\beta\left(\frac{v_0}{\alpha}\right)-2\gamma-k(k+1);\quad \beta=\frac{(E+Mc^2)}{\hbar^2c^2\alpha^2},\gamma=\frac{(E^2-M^2c^4)}{\hbar^2c^2\alpha^2}$$

$$\chi_0=-\gamma \tag{24}$$

Comparing Eqn. (23) with Eqn. (2), we can easily obtain the coefficients ε_i (i = 1, 2, 3) as follows:

$\varepsilon_1=\varepsilon_2=\varepsilon_3=1$ (25)

The values of the coefficients ε_i (i = 4, 5 …13) are also found from Eqn. (9) and Eqn. (10) as below in Table 1.

Table 1.The coefficients ε_i (i = 4, 5 …13)

$\varepsilon_1=\varepsilon_2=\varepsilon_3=1$	$\varepsilon_4=0$	$\varepsilon_5=-\frac{1}{2}$
$\varepsilon_6=\chi_2+\frac{1}{4}$	$\varepsilon_7=-\chi_1$	$\varepsilon_8=\chi_0$
$\varepsilon_9=\chi_2-\chi_1+\chi_0+\frac{1}{4}$	$\varepsilon_{10}=2\sqrt{\chi_0}$	$\varepsilon_{12}=\sqrt{\chi_0}$
$\varepsilon_{11}=2\sqrt{\chi_2-\chi_1+\chi_0+\frac{1}{4}}$	$\varepsilon_{13}=\frac{1}{2}+\sqrt{\chi_2-\chi_1+\chi_0+\frac{1}{4}}$	

Using the energy equation, Eqn. (5) for energy Eigen-values we have:

$$(2n+1)\left[\sqrt{\eta_2-\eta_1+\eta_0+\frac{1}{4}}+\sqrt{\eta_0}+\frac{1}{4}(2n+1)\right]$$

$$+2\sqrt{\eta_0(\eta_2-\eta_1+\eta_0+\tfrac{1}{4})}+2\eta_0-\eta_1+\tfrac{1}{4}=0 \tag{26}$$

Let us find the corresponding wave functions. In reference to Eqn. (6), Eqn. (7) and using of the coefficients ε_i in Table 1, we can obtain the upper wave function

$$F_{n,k}(r)=\frac{N}{r}(e^{-\alpha}\ )^{\sqrt{\chi_0}}(1-e^{-\alpha r})^{(\sqrt{\chi_2-\chi_1+\chi_0+\frac{1}{4}}+\frac{1}{2})} \times P_n^{(2\sqrt{\chi_0},2\sqrt{\chi_2-\chi_1+\chi_0+\frac{1}{4}})}(1-2e^{-\alpha r} \tag{27}$$

Where N is the normalization constant, on the other hand, the lower component of the Dirac spinor can be calculated from Eqn. (28) as

$$G_{n_r,k}(r)=\frac{\hbar^2c^2}{E+Mc^2}\left(\frac{d}{dr}+\frac{k}{r}\right)F_{n_r,k}(r) \tag{28}$$

And wave function for Dirac equation can be calculated from Eqn. (29) as

$$\psi_{n_r,k}(r,\theta,\phi) = N\begin{bmatrix} Y_{jm}^{l}(\theta,\phi) \\ \frac{i}{[M+E_{n_r,k}]}\left[\frac{d}{dr}+\frac{k}{r}\right]Y_{jm}^{\tilde{l}} \end{bmatrix}(e^{-\alpha r})^{\sqrt{\chi 0}} \times(1-e^{-\alpha r})^{\sqrt{\chi 2-\chi 1+\chi 0+\frac{1}{4}}+\frac{1}{2}}P_n^{(2\sqrt{\chi 0},2\sqrt{\chi 2-\chi 1+\chi 0+\frac{1}{4}})} \times(1-2e^{-\alpha r}) \tag{29}$$

4.2 Calculation of charge radius and electric quadrupole moment

The radial wave function is obtained from equation (29), so we can easily calculate the charge radius of studied isotopes by calculating $<r^2>^{1/2}$ by using of the Eqn. (29) and Eqn. (30).

$$\langle r^2\rangle^{\frac{1}{2}}=\left(\frac{\int\psi^*_{n_r,k}(r)r^2\psi_{n_r,k}(r)d^3r}{\int\psi^*_{n_r,k}(r)\psi_{n_r,k}(r)d^3r}\right)^{\frac{1}{2}} \tag{30}$$

The nuclear electric quadrupole moment is a parameter which describes the effective shape of the ellipsoid of nuclear charge distribution. A non-zero quadrupole moment Q indicates that the charge distribution is not spherically symmetric.

When the neutron or proton number is close to the full layer, the nucleus basically is spherical. Therefore, in this region for odd-A nuclei, the electric quadrupole moment (Q) is essentially determined by the nucleon with the odd number. So, we expect that if the difference between the neutron number or proton number, with the full layer in a nucleus is equal to one, the equations for this nucleus below will be correct. Of course, by considering this point that if there is a single cavity in the shell, so Q is positive and if there is an extra particle in addition to the full layer, Q is negative.

$$Q=\frac{3K^2-I(I+1)}{(I+1)(2I+3)}Q_0,\quad Q_0=\frac{3}{\sqrt{5\pi}}ZeR^2\beta \tag{31}$$

The quantity Q_0 is the classical form of the calculation represents the departure from spherical symmetry in the rest frame of the nucleus. The expression for Q is the quantum mechanical form which takes into account the nuclear spin I and the projection K in the z-direction. For the ground state of an odd-A nucleus that I=K, the above equation is converted to the following equation where β is the deformation parameter.

$$Q=\frac{I(2I-1)}{(I+1)(2I+3)}Q_0 \tag{32}$$

5. Results and discussion

We consider ^{41}Ca and ^{17}O isotopes with a single nucleon on top of the ^{40}Ca and ^{16}O isotopes core. Since these isotopes have one nucleon out of core, these isotopes could be considered as single particle model in relativistic shell model. Relativistic mean field (RMF) theory, as a covariant density functional theory, has been successfully applied to the study of nuclear structure properties [15]. The RMF theory incorporates from the beginning very important relativistic effects, such as the existence of two types of potentials (Lorentz scalar and four-vector) and the resulting strong spin-orbit interaction, a new saturation mechanism by the relativistic quenching of the attractive scalar field, and the existence of antiparticle solutions. Therefore, it is interesting to apply RMF theory to investigate the binding energy difference of mirror nuclei [16]. So we could use of Dirac equation for investigation them. The ground state and first excited energies of ^{41}Ca and ^{17}O isotopes are obtained by using Eq.(26). These results are compared with the experimental data in Table 2 [17].

Table 2. Ground state energy of ^{41}Ca and ^{41}Sc isotopes

Isotope	Parameters of modified potential			state	E_{our} (MeV)	E_{exp} (Mev) [17]
	$\alpha(fm^{-1})$	V_0	V_1			
^{41}Ca	0.069	47.8647	11.2182	$1f_{7/2}$	-350.8092	-350.4148
^{17}O	0.069	26.2284	4.4772	$1d_{5/2}$	-132.0443	-131.7624

The calculated energy levels have good agreement with experimental values. Therefore, the proposed model can well be used to investigate other similar isotopes. We obtain the charge radius by using Eqn. (29) and Eqn. (30) and electric quadrupole moment by using Eqn. (32) for ^{41}Ca and ^{17}O isotopes. In Table 3 we show the charge radius and electric quadrupole moment for ground state ^{41}Ca and ^{17}O isotopes and compare with experimental data and others work. We consider β=0.08 for ^{41}Ca and β=0.17 for ^{17}O isotopes.

Table 3. Charge radius and the electric quadruple moment for ^{41}Ca and ^{41}Sc isotopes for ground state energy

	charge radius		Quadrupole moment	
Isotope	Our work	Experimental [18]	Our work	Experimental [19]
^{41}Ca	3.4560	3.4780	6.7505	6.65
^{17}O	2.6769	2.6932	2.6346	2.56

The charge radius obtained for ground state ^{41}Ca and ^{17}O isotopes has good agreement with experimental value. We can also predict the electric quadruple moment for ^{41}Ca and ^{17}O isotopes. These results show that our model could be useful to check other similar isotopes which can be investigated in a similar way.

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