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Calculation of Ground State Energies of Even-Even Isotopes with Nuclear Models

[1]J. Khosravi Bizhaem and [2]M. R. Shojaei

[1] *Department of physics, Shahrood University of Technology, Iran, e-mail: khosravi_1224@yahoo.com*
[2] *Department of physics, Shahrood University of Technology, Iran, e-mail: shojaei.ph@gmail.com*

Relativistic theory has been successful in describing nuclear phenomena. Therefore, this article investigated shell and cluster models in a relativistic manner. In this regards, considering appropriate potential for a few-body system by Jacobean coordinate, Klein-Gordon equation was solved by Nikiforov-Uvarov method. Then ground state energy and the first excited state of several light nuclei were calculated and compared with experimental values, which showed the efficiency of this model for investigation of energy levels of different nuclei.

1. Introduction

There is no complete theory which describes the structure and behavior of complex nuclei. Conceptual models however have been designed for understanding the physics of such inherently complex states. These models involve certain aspects of our understanding and simplify the calculations by simple assumptions. One of the simplest nuclear models is the liquid droplet model, in which the nucleus is regarded as a series of neutrons and protons gathered as an incompressible droplet [1]. Failures of this model resulted in development of shell model in which most of the nucleons form a neutral central part, and only a few of them can be found outside this central region producing low-energy excited states.

This model managed to predict a large range of nuclear observables such as spin and parity, for nuclear levels. In fact, the structure of atomic nuclei is described as energy levels which follow the exclusion principle of Pauli. This theory is based on this principle that each nucleon moves independently in the average potential due to the interaction of other nucleons in the nucleus. [2, 3] This requires that light nuclei with a half-filled shell appear as elliptical nuclei [4]. Deformation of light nuclei is not only observed in axial deviations, but it also creates a cluster structure. It should be noted that in most nuclei, there is no cluster structure in the ground state and it appears by increase of nuclear internal energy. Accordingly, some combinations of nucleons exist in the nucleus and interact with each other while maintaining themselves. The merits of examining the nuclear structure with cluster model will be highlighted when the relative motion between the clusters becomes the main state of the nucleus.

There is an extreme for clustering behavior for A = 4n nuclei, in which the whole nucleus does not behave like a liquid droplet, but it rather acts as a condensation of n individual alpha-like droplets [5, 6], when excessive excitement energy is added to these nuclei, the configuration of their central mass may be separated and expanded in space. Limiting cases are linear chain states which were predicted in a wide range of masses [7].

To examine the nuclei in each of these nuclear models, we will encounter with a many-body system. One of the methods widely used for investigation of such systems is application of phenomenological potentials. In this method, appropriate potential with several parameters will be considered for the interactions between particles of a system. Then, by examining the experimental results, the parameters will be chosen in such a way that the greatest agreement could be achieved between the theory and the experimental results [8, 9].

Over the past three decades, relativistic theory has been successful in describing nuclear phenomena of unstable nuclei as well as stable ones. In comparison with non-relativistic theories, relativistic theory can reproduce real properties of nuclear saturation in a nuclear material. The main feature of the relativistic nuclear dynamics is the emergence of scalar gravity fields of S and vector repulsion of V which provide the ability to simultaneously unify the attractive and repulsive effects of long and short distances in nuclear interactions, and reflect the possibility to use relativistic nuclear dynamics for further modifications in the nuclei structure [10-13]. In this context, the present paper investigated the shell and cluster models by relativistic methods considering a proper central potential. By solving the Klein-Gordon equation by Nikiforov-Uvarov method and obtaining the Eigenvalue equations of energy, we examine the efficacy of our model through comparing experimental and computational results for several isotopes.

2. Review of Nikiforov-Uvarov Method

Klein-Gordon equation was converted to following from after selecting proper variable of s=s(r) [14].

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

Where, $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of at most second order and $\tilde{\tau}(s)$ is a polynomial which can be first order at most. Considering $\Psi_n(s)$ as a multiplication

:

$$\Psi_n(s)=\varphi_n(s)y_n(s) \tag{2}$$

Equation 1 can be reduced to a hyper-geometrical equation as:

$$\sigma(s)y''_n(s)+\tau(s)y'_n(s)+\lambda y_n(s)=0 \tag{3}$$

In which $\tau(s)=\tilde{\tau}(s)+2\pi(s)$, and $\tau'(s)<0$ should also hold. This means that first derivative of $\tau(s)$ should be negative. λ is a parameter defined as follows and setting the equations in 4 equal results in energy Eigen values :

$$\begin{cases}\lambda_n=-n\tau'(s)-\dfrac{n(n-1)}{2}\sigma''(s), \\ \lambda=K+\pi'(s)\end{cases} \qquad (n=0,1,2,\ldots) \tag{4}$$

It must be mentioned that λ and λ_n will be obtained from a specific solution, $y(s)=y_n(s)$, obtained from a n-order polynomial. Moreover, the term $y_n(s)$ is the wave function of equation 2 which is a hypergeometric function obtained from Rodriguez equation

$$y_n(s)=\frac{B_n}{\rho_n}\frac{d}{ds^n}(\sigma^n(s)\rho(s)) \tag{5}$$

In this equation, B_n is normalization constant and $\rho(s)$ is a weight function which satisfies the following condition:

$$\frac{d}{ds}\omega(s)=\frac{\tau(s)}{\sigma(s)}\omega(s) \qquad \omega(s)=\sigma(s)\rho(s) \tag{6}$$

$\pi(s)$ is defined as:

$$\pi(s)=\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\pm\sqrt{\left(\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\right)^2-\tilde{\sigma}(s)+K\sigma(s)} \tag{7}$$

As should be a first order polynomial at most, term underneath the radical in equation 7 should be set as first order polynomial. In this way, $\Delta=b^2-4ac$ can be equal to zero. In such cases, an equation will be obtained for K whose values can be substituted in equation 7. Comparing it with equation 4, energy eigenvalues will be obtained.

3. The Klein–Gordon Equation in (D+1) Dimensions

The D-dimensional time-independent arbitrary l-states radial Klein-Gordon equation with scalar and vector potentials *S(r)* and *V(r)*, where *r*=|*r*| is describing a spin-less particle (such as α particle), takes the general form [15, 16]:

$$\nabla_D^2\Psi_{\ell_1\ldots\ell_{D-2}}^{\ell_{D-1}-1}\left(r\right)+\frac{1}{\hbar^2c^2}\left\{\left[E_{n,\ell}-V\left(r\right)\right]^2-\left[Mc^2+S\left(r\right)\right]^2\right\}\Psi_{\ell_1\ldots\ell_{D-2}}^{\ell_{D-1}-1}\left(r\right)=0\Big\} \tag{8}$$

$$\nabla_D^2\Psi_{\ell_1\ldots\ell_{D-2}}^{\ell_{D-1}-1}\left(r\right)+\frac{1}{\hbar^2c^2}\left\{\left[E_{n,\ell}-V\left(r\right)\right]^2-\left[Mc^2+S\left(r\right)\right]^2\right\}\Psi_{\ell_1\ldots\ell_{D-2}}^{\ell_{D-1}-1}\left(r\right)=0\Big\} \tag{8}$$

We define a set of Jacobi coordinates for which $\zeta_N=r_{ij}$. The center of mass R can be eliminated by using the Jacobi coordinates:

$$\zeta_i=\sqrt{\frac{i}{i+1}}\left(r_{i+1}-\frac{1}{i}\sum_{j=1}^{i}r_j\right), i=1,\ldots,N-1 \tag{9}$$

Where

$$\begin{aligned}x^2&=\sum_{i=1}^{N-1}\left(\zeta_i^2\right)=\sum_{i=1}^{N-1}\left(r_i-R\right)^2=\frac{2}{N-1}\sum_{k;\ell\rangle k}r_{k\ell}^2\\ R&=\frac{1}{N}\sum_{i}^{N}r_i\end{aligned} \tag{10}$$

The N-body problem in the center-of-mass frame is mathematically (*3N-3*) - dimensional. In the hyper-spherical method, a point in the (*D=3N-3*)-dimensional configuration space is represented as lying on a (*D-1*)-dimensional hyper-sphere of radius *x* [17]. In addition, ***x*** is a D-dimensional position vector in Jacobi coordinates.

The Laplace operator written in hyper-spherical coordinates in the D-dimensional space for N identical particles becomes [18-20]

$$-\sum_{i=1}^{N-1}\nabla_{\zeta_i}^2 = -\sum_{i=1}^{N-1}\nabla_x^2 = -\left(\frac{d^2}{dx^2}+\frac{D-1}{x}\frac{d}{dx}+\frac{L^2(\Omega)}{x^2}\right) \tag{11}$$

Applying the separation variable method by means of the solution,

$$\psi_{n\ell m}(x,\Omega_D) = U_{n\ell}(x)Y_\ell^m(\Omega_D) \tag{12}$$

Eq. (12) provides two separate equations, Where $Y_\ell^m(\Omega_D)$ is known as the hyper-spherical harmonics.

$$L^2(\Omega)Y_\ell^m(\Omega_D) = \ell(\ell+D-2)Y_\ell^m(\Omega_D) \tag{13}$$

In the case that the scalar and vector potential have equal magnitudes, *V(x) = S(x)* by Jacobi relative considerations, the time-independent hyper-radial Schrödinger-like equation in D-dimensions [21] becomes:

$$\left\{\frac{d^2}{dx^2}+\frac{D-1}{x}\frac{d}{dx}-\frac{\ell(\ell+D-2)}{x^2}+\frac{(E^2-M^2c^4)}{\hbar^2c^2}-2\frac{(E+Mc^2)}{\hbar^2c^2}V(x)\right\}U_{n\ell}(x)=0 \tag{14}$$

The quadratic Hellmann potential is defined as [22, 23]:

$$\mathrm{V(x)} = -\frac{\mathrm{a}}{\mathrm{x}}+\frac{\mathrm{b}}{\mathrm{x}^2}\mathrm{e}^{-\alpha \mathrm{x}} \tag{15}$$

Where, the parameters *a* and *b* are real parameters, these are strength parameters, and the parameter α is related to the range of the potential.

Equation (14) is exactly solvable only for the case of *l=0*. In order to obtain the analytical solutions of Eq. (14), we employ the improved Pekeris approximation [24] that is valid for $\mathrm{e}^{-\alpha \mathrm{x}}$. The main characteristic of these solutions lies in the substitution of the centrifugal term by an approximation, so that one can obtain an equation, normally hypergeometric, which is solvable [25, 26].

$$\frac{1}{\mathrm{x}^2} \approx \frac{\alpha^2}{(\mathrm{e}^{-\alpha \mathrm{x}}-1)^2} \tag{16}$$

Also this approximation in reverse order could be used.

We can write the Eq. (14) by using improved Pekeris approximation as summarized below:

$$U''_{n,\ell}(x)+\frac{(D-1)}{x}U'_{n,\ell}(x)+\frac{1}{x^2}\left[-\eta_2 s^2+\eta_1 s-\eta_0\right]U_{n,\ell}(x)=0 \tag{17}$$

Where the parameters η_2, η_1 and η_0 are considered as follows:

$$\begin{aligned}&\eta_2=\left[2\beta\alpha^2 b-\gamma\right]\\ &\eta_1=2\beta\left[a+b\alpha\right], \qquad \gamma=\frac{\left(E^2-M^2c^4\right)}{\hbar^2c^2},\quad \beta=\frac{\left(E+Mc^2\right)}{\hbar^2c^2}\\ &\eta_0=2\beta b+\ell\left(\ell+D-2\right)\end{aligned} \tag{18}$$

Applying NU method, we obtain the energy equation as:

$$(2n+1)\sqrt{\eta_2}-\eta_1+2\sqrt{\eta_2\left[\frac{(2-D)^2}{4}+\eta_0\right]}=0 \tag{19}$$

Finally, considering the notations of Eqns. (18) and (19), the equation of energy can be obtained as:

$$\sqrt{\frac{\left(E+Mc^2\right)}{\hbar^2c^2}\left[2\alpha^2 b-\left(E-Mc^2\right)\right]}\left\{\begin{array}{l}(2n+1)+\\ 2\sqrt{\frac{(2-D)^2}{4}+2b\frac{\left(E+Mc^2\right)}{\hbar^2c^2}+\ell\left(\ell+D-2\right)}\end{array}\right\} -\left[2a+2\alpha b\right]\frac{\left(E+Mc^2\right)}{\hbar^2c^2}=0 \tag{20}$$

And the hyper-radial wave function can be written in the bellow form:

$$U_{n,\ell}(x)=Nx^{\frac{(2-D)}{2}+\sqrt{\frac{(2-D)^2}{4}+\eta_0}}e^{-\sqrt{\eta_2}x}L_n^{2\sqrt{\frac{(2-D)^2}{4}+\eta_0}}\left(2\sqrt{\eta_2}x\right) \tag{21}$$

Where, *N* is the normalization constant.

4. Result and Discussion in Shell Model

We investigate a systematic study of both nuclear binding energies and excited energies in (even) oxygen isotopes ^{18}O and ^{20}O. We have investigated energy levels these isotopes in Relativistic Shell model. These isotopes can be considered as a doubly-magic close shell ^{16}O with additional nucleons (valence) in the $ld_{5/2}$ level. Then, using the Jacobi coordinate transformation in hyper-spherical approach, the relativistic Klein–Gordon equations under spin symmetry in D-dimensional are investigated for quadratic Hellmann potential for interaction between core and additional nucleons. Using Parametric Nikiforov-Uvarov method, we have calculated the energy levels and wave function in Kline-Gordon equation in relativistic shell model. Finally, we have computed the binding and excited energy levels for these isotopes and compare with other works. Our results were in agreement with experimental values and hence this model could be applied for similar nuclei.

We consider (even) oxygen isotopes ^{18}O and ^{20}O as a doubly-magic close shell ^{16}O with additional nucleons (valence) in the $ld_{5/2}$ level. We have investigated energy levels these isotopes in Relativistic Shell model. Then, using the Jacobi coordinate transformation in hyper-spherical approach and Parametric Nikiforov-Uvarov method, we have calculated the energy levels and wave function in Kline-Gordon equation 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 [27]. Therefore, it is interesting to apply RMF theory to investigate the binding energy difference of mirror nuclei [28]. So we could use of K-G equation for investigation them. The ground state and first excited energies of (even) oxygen isotopes ^{18}O, ^{20}O are obtained in relativistic shell model by using Eq. (20). These results for relativistic shell model are compared with the experimental data and others work in table 1.

Table 1
The ground state and the first excited energy of (even) oxygen isotopes ^{18}O and ^{20}O in Relativistic shell model (with α=0.012fm^{-1}).

Isotope	a	b	state	E_{-Our}(MeV)	E_{-Other}(MeV)[29]			E_{Exp}(MeV) [30]
					NL3	NL-Z2	NL-BA	
^{18}O	127.3849	1.3487	$(0^+)_1$	-139.8993	141.101	140.643	139.909	139.8087
			$(2^+)_1$	-137.9258	-	-	-	137.8266
^{20}O	142.4517	3.6049	$(0^+)_1$	-151.3033	152.300	152.161	151.247	151.3714
			$(2^+)_1$	-149.6265	-	-	-	149.6977

The calculated energy levels have good agreement with experimental values. Therefore, the proposed model can well be used to investigate other similar isotopes and compare with experimental data.

In [31], we have investigated the ground state energy of oxygen isotopes by Hult'en plus Yukawa potential as interaction between particles in Non-Relativistic system [31]. In this work, we have obtained better agreement with experimental values comparing pervious paper.

5. Result and Discussion in Cluster Model

Regarding relatively good agreement between the computed and experimental energy levels in shell model, in this section we investigated the relativistic cluster model with quadratic Hellman potential and examined the results for ground and first excited state of some light alpha-conjugated nuclei.

^{8}Be isotope is the simplest system for investigating this model; this isotope includes two alpha particles. Ikida diagram predicts that the cluster structure can be observed in the threshold of decay or a little lower. Regarding low half- life of this isotope (~ 10^{-16} s), alpha structure cluster can be seen in ground state.

The binding energy of ^{8}Be isotope is -57/75 MeV, and its ground state level decays into two alpha particles by receiving 92keV energy; its first excited level, +2, also has the energy of -53.27 MeV. Now, using equation (20) and selecting the most suitable potential coefficients, we calculated the amount of ground state energy and the first excited level of this isotope, which was compared with experimental values in Table 2.

The next examined systems that were ^{12}C and ^{16}O isotopes. In Hoyle's excited equilibrium, 2+, ^{12}C has a cluster structure consisting of three alpha particles. ^{16}O isotope has 8 protons and 8 neutrons; and according to the shell model, it has two 1P $_{1/2}$ packets and two magic pockets. Ikida's diagram predicts that ^{16}O isotope has two-cluster structure of ^{12}C + α at energy of -120/46 MeV and four-alpha clusters at 183.11 MeV [5], [6]. Experimental results also confirmed Ikida's prediction. When the excitement energy of nucleus reaches to -184.19 MeV, it gets 3-cluster structure and eventually at -169.76MeV, it will have a structure consisting of six alpha particles. Now, after determining the coefficients by fitting on the clustered system, the calculated results for the ground state and the first excited level of all isotopes are listed in Table 2.

Table2

The ground state and the first excited energy for A=4n isotopes in Relativistic cluster model (with α=0.012fm^{-1}).

			E$_{\text{-Other}}$(MeV)[29]			
Isotope	**state**	**E$_{\text{-Our}}$(MeV)**	**NL3**	**NL-Z2**	**NL-BA**	**E$_{\text{-Exp.}}$(MeV)[30]**
^{8}Be	$(0^{+})_1$	-139.8993	141.101	140.643	139.909	139.8087
	$(2^{+})_1$	-137.9258	-	-	-	137.8266
^{12}C	$(0^{+})_1$	-151.3033	152.300	152.161	151.247	151.3714
	$(2^{+})_1$	-149.6265	-	-	-	149.6977
^{16}O	$(0^{+})_1$	-162.1292	163.173	163.082	162.159	162.0300
	$(2^{+})_1$	-158.9363	-	-	-	158.8310

As tables 1 and 2 suggest, relativistic shell model was successful in investigation of isotopes possessing a central nucleus and extra nucleons acting as valance nucleons. It can be also used for other isotopes. Moreover, relativistic cluster model is the most suitable one for isotopes with A=4n in which n shows the number of alpha particles

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