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ARTICLE

Calculation of the Electric Quadrupole Moment of ^6Li and ^7Li in Shell Model and Cluster Model

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Abstract: In this paper, we have investigated electric quadrupole moment of the ^6Li and ^7Li in both shell model and cluster model. In shell model, the nuclei ^6Li and ^7Li can be modeled as one core plus nucleons, Nucleons outside the closed shell can be considered as a two- and three-particle system. In cluster structure, we have selected alpha clusters and triton or deuteron in interaction with alpha cluster (^7Li and ^6Li involving $\alpha + {}^3H$ and $\alpha + {}^2H$ respectively). By solving Schrodinger equation and using suitable potential for interaction between particles by applying Nikiforov-Uvarov method, potential coefficients have been computed. Then we have calculated the energy and wave function for nuclei ^6Li and ^7Li and compare with experimental results. By having the wave function we can obtain quadrupole. These values are compared with predictions from shell-model and cluster-model calculations. Although the difference between them is too small but the electric quadrupole moment results in the cluster model are in good agreement with experimental results.

Keywords: Electric quadrupole moment, Shell-model, Cluster-model, *Li* isotopes, Non-relativistic equation.

Introduction

Electric quadrupole and magnetic dipole moments can be determined using an experimental method that is based on the nuclear magnetic resonance technique [1, 2, 3]. In nuclear physics, the study of isotopes and calculation of static properties in the different models are the main goal. The most important models in nuclear physics are shell and cluster models. Shell model is an acceptable in nuclear physics, ^7Li and ^6Li are described in the shell model with p-shell wave functions. Cluster structure in nuclear means that the nucleus behaves as a combination of clusters, and cluster means infrastructures with a specific spatial position that are composed of nucleons with strong correlations In the theoretical point of view, the energy of Li isotopes have been studied in many different ways [1, 4]. C. Forssen and *et al.* calculated the charge radii and electromagnetic moments of the A ≤ 11 chains of Li and Be isotopes. They compared the performance of two very different NN interactions: (1) the CD-Bonn 2000 interaction (CDB2k) [5], that is a charge-dependent NN interaction based on one-boson exchange; and (2) the INOY IS-M [6] that is a phenomenological interaction for which non-locality was introduced in certain partial waves so that the binding energies of ^3H and ^3He are described correctly [1]. It is very useful to describe a suitable model consistent with experience in different trends in physics to solve problems. In nuclear physics, due to the complexity of the potentials, a model must be considered in order to overcome this complexity. In different nuclear models, cluster model and shell model have considerable answers for

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nuclei, especially light nuclei. Since the wave function contains a lot of necessary information for descriptions of quantum system, so solving equations such as Schrödinger equation in nonrelativistic quantum mechanics is very important [7]. The lithium isotopes have received much attention due to its rich experimental results in static properties. Recent studies have investigated some of the static properties of lithium isotopes, such as charge radius, energy spectrum, and electrical quadrupole moment that present a good picture of their nuclear structure. It is useful to calculate these quantities to test microscopic theory by future experiments [1, 8, 9, 10]. In this work we calculated electric quadrupole moment of ^{7}Li and ^{6}Li in two ways: cluster model and shell model. By selecting a suitable potential in the cluster and shell model, Ground-state binding energies and wave function and finally quadrupole of lithium isotopes by solving the non-relativistic equation (Schrodinger) are investigated. In the cluster model, which has recently been considered by many researchers, nucleons are considered as clusters that reduce the complexity of multiparticle systems. The alpha cluster consists of two protons and two neutrons [11]. ^{7}Li And ^{6}Li involving $\alpha + {}^{3}H$ and $\alpha + {}^{2}H$ respectively, which form a two-particle system. In shell model, we consider ^{4}He as a closed shell plus few nucleons outside the closed shell .Nucleons outside the closed shell can be considered as a two- and three-particle system then we calculated electric quadrupole moment. The results obtained from the calculations in these models compare with the experimental data and other results [1, 2, 3].. To calculate the electric quadrupole moment, we need the wave function of the system, so we use the Schrodinger equation and solve it for these models and then we obtained Ground-state binding energies and wave functions.

The cluster model is one of the most important describing in many-particle systems in nuclear models. Studying the properties of many-particle systems is complex and difficult due to its high degrees of freedom, so the cluster model is one of the useful solutions to solve this problem, Instead of investigated individual particles, we consider the interaction between clusters. According to the cluster model, the nucleus are a combination of subsystems with a specific spatial position composed of strongly correlated nucleons. One of the most important clusters is the alpha cluster.

In the shell model, the nucleus energy levels are considered as layers and sublayers in which the nucleons are define. In the layered model, using the Pauli Exclusion Principle, the structure of the nucleus is expressed based on energy levels, which has been successful in predicted in magic numbers. Evidence for the validity of the shell model comes from experimental observations such as binding energy, spin, and so on.

Schrodinger Equation in Cluster Model

To investigate of the nuclei are used two perspectives: relativistic and non-relativistic, each of them is particular importance. In this work, we use a non-relativistic system. In non-relativistic quantum mechanics, the Schrodinger equation is as follows:

$$H\psi = E\psi,$$

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right\}\psi_{n.l}(r) = E_{n,l}\psi_{n.l}(r)$$

where H is the Hamiltonian system and E is the energy system.

For a two-cluster system, the Schrödinger equation for the radial potential V(r) has the following form [12, 13]:

$$\frac{-\hbar^2}{2\mu}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\psi_{n.l}(r) + (V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2})\psi_{n.l}(r) = E_{n,l}\psi_{n.l}(r) \quad (1)$$

The first step of studying the properties of nuclei in shell model and also cluster model is choosing a suitable potential [14]. In this reason, in cluster structure the phenomenological interaction potential between α-clusters is considered as:

$$V(r) = V_0\frac{e^{-2\alpha r}}{r^2} + \frac{b}{r^2}e^{-\alpha r} \quad (2)$$

Yukawa potential is one of the most important potential which has been studied by many researchers in physics and chemical physic [15, 16, 17]. In this work we use inversely quadratic Yukawa (IQY) potential and Due to nuclear force saturation at lower distances, one add a repulsive term to plus repulsive term potential as interaction between particles and clusters. V_0 is the parameter describing the

potential well depth, the α representing the potential range and b is adjustable parameter. By substituting the Eq. (2) in Eq. (1), the radial Schrödinger equation is obtained as:

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}-\frac{l(l+1)}{r^2}+\frac{2\mu}{\hbar^2}\left[E-V_0\frac{e^{-2\alpha r}}{r^2}-\frac{b}{r^2}e^{-\alpha r}\right]R=0 \quad (3)$$

Then, with further analysis and simplification, Eq. (3) becomes:

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+\frac{1}{r^2}[-\varepsilon^2r^2-\beta r-\gamma]R=0,$$
$$\begin{cases} -\varepsilon^2=\frac{2\mu}{\hbar^2}E \quad \varepsilon>0 \\ l(l+1)+\frac{2\mu}{\hbar^2}(V_0+b)=\gamma \\ \frac{2\mu}{\hbar^2}(\alpha b+2V_0\alpha)=-\beta \end{cases} \quad (4)$$

It is seen from Eq. (4) that the equation has the exponential square and inverse radial square terms, which cannot be solved analytically then we use NU method. At this point, we briefly describe the NU method

The General Framework of the Nikiforov–Uvarov (NU) Technique

The Nikiforov–Uvarov method offers a powerful mathematical model to solve second-order differential equations [18]. For a given potential, the Schrödinger equations reduced to a generalized equation of hypergeometric type with an appropriate coordinate trans-formation *s* = *s*(*r*). In this method the differential equations can be written in the following form [19, 20]:

$$\psi''_n(s)+\frac{\tilde{\tau}(s)}{\sigma(s)}\psi'_n(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s)=0 \quad (5)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials that can be at most second degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. To find a particular solution for Eq. (4) by separation of variables, we have the following trans- formation:

$$\psi(s)=\varphi(s)y(s) \quad (6)$$

It reduces Eq. (5) to a hyper-geometric type function:

$$\sigma(s)y''(s)+\tau(s)y'(s)+\lambda y(s)=0 \quad (7)$$

where $\tau(s)=\tilde{\tau}(s)+2\pi(s)$ and $\tau'(s)<0$ which means $\tau(s)$ has a negative derivative. Additionally, λ is a parameter with the following definitions:

$$\begin{cases} \lambda_n=-n\tau'(s)-\frac{n(n-1)}{2}\sigma''(s),\ n=0,1,2,\dots \\ \lambda=k+\pi'(s) \end{cases} \quad (8)$$

And equality of the two parts in Eq. (8) yields the energy eigenvalues of the intended multi-particle system.

$\pi(s)$ is a polynomial with the parameter s and the determination of k is the essential point in the calculation of $\pi(s)$. In order to find the value of k, the expression under the square root must be square of a polynomial

$$\pi(s)=\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\pm\sqrt{\left(\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\right)^2-\tilde{\sigma}(s)+k\sigma(s)} \quad (9)$$

The function $\varphi(s)$ is defined as a logarithmic derivative

$$\frac{\varphi'(s)}{\varphi(s)}=\frac{\pi(s)}{\sigma(s)} \quad (10)$$

y(*s*) is the hypergeometric type function whose polynomial solutions are given by Rodrigues relation:

$$y_n(s)=\frac{B_n}{\rho_n}\frac{d^n}{ds^n}(\sigma^n(s)\rho(s)) \quad (11)$$

B_n is the normalizing constant and the weight function ρ must satisfy the following condition:

$$(\sigma\rho)'=\tau\rho \quad (12)$$

Mathematical Calculation and Results

If we apply the NU method based on the discussed model, by comparing (4) and (5), the following expressions are obtained:

$$\tilde{\tau}=2,\ \sigma=r,\ \sigma^2=r^2,\ \tilde{\sigma}=-\varepsilon^2r^2-\beta r-\gamma \quad (13)$$

Substituting the above expression into (8), and considering the NU method condition for $\pi(s)$ with some analysis and simplification, the following equation can be achieved:

$$\pi(r)=-\frac{1}{2}-\frac{1}{2}(2\varepsilon r\pm\sqrt{1+4\gamma}\,) \quad (14)$$

Since we have the polynomial $\tau(s)=\tilde{\tau}(s)+2\pi(s)$ with a negative derivative, the suitable form has to be established for this parameter. We have:

$$\tau=1-(2\varepsilon r-\sqrt{1+4\gamma}\,) \quad (15)$$

Finally, considering the notations of (8) and Eq. (4), we can write the energy Eigen-values for such a system of α-clusters as:

$$E = -\frac{2\mu}{\hbar^2}\frac{(\alpha b+2V_0\alpha)^2}{\left[2n+1+\sqrt{1+4l(l+1)+\frac{2\mu}{\hbar^2}(V_0+b))}\right]^2} \quad (16)$$

By using $\psi(s) = \varphi(s)y(s)$, the solution of (4) can be written as the wave function of the Schrodinger equation as follow:

$$\psi = B_n r^{-\frac{1}{2}+\sqrt{1+4\gamma}}\exp(-\varepsilon r)L_n^{\sqrt{1+4\gamma}}(2\varepsilon r) \quad (17)$$

where, B_n is the normalization constant. We have obtained the potential parameters by fitting the ground state energy for mentioned isotopes. In this way, the chosen parameters are for ^6Li in which both n and l are set to 1, $V_0 = 42.3\ MeV$, $b = 1.7\ MeV$, $\alpha = 0.00125\ fm^{-1}$ and for ^7Li $V_0 = 35MeV$, $b = 1.15MeV$, $\alpha = 0.00158fm^{-1}$. The values of ground states binding energies are shown in table 1.

Schrodinger Equation in Shell Model

Studying the nucleon-nucleon interactions is very useful to find the many important properties of multi-nucleon systems. In this section we select a core and considering the Eq. (2) for the interaction between nucleons. To study the energy spectrum and wave function for N-body system, we use the time independent Schrödinger equation [12-21]. That is as follow

$$\frac{d^2R}{dr^2}+\frac{D-1}{r}\frac{dR}{dr}+\frac{2\mu}{\hbar^2}\left[E - V_0\frac{e^{-2\alpha r}}{r^2}-\frac{b}{r^2}e^{-\alpha r} - \frac{\hbar^2}{2\mu}\frac{l(l+D-2)}{r^2}\right]R = 0 \quad (18)$$

where $R(r)$ and $V(r)$ are the radial parts of the N-body wave function and the potential, respectively in eq. (2), $D = 3N - 3$ and μ is the reduced mass. E represents the energy of the system. In order to solve the above equation, we have

$$\frac{d^2R}{dr^2}+\frac{D-1}{r}\frac{dR}{dr}+\frac{1}{r^2}\left[\frac{2\mu}{\hbar^2}Er^2-\frac{2\mu}{\hbar^2}V_0 + \frac{2\mu}{\hbar^2}V_0(2\alpha r)-\frac{2\mu}{\hbar^2}b+\frac{2\mu}{\hbar^2}b\alpha r - l(l+D-2)\right]R = 0 \quad (19)$$

Then, with further simplification, Eq. (18) becomes:

$$\frac{d^2R}{dr^2}+\frac{D-1}{r}\frac{dR}{dr}+\frac{1}{r^2}[-\varepsilon^2r^2-\beta r-\gamma]R = 0,$$

$$\begin{cases}\frac{2\mu}{\hbar^2}(V_0+b)+l(l+D-2)=\gamma\\ \frac{2\mu}{\hbar^2}(2\alpha V_0+b\alpha)=-\beta\\ \frac{2\mu}{\hbar^2}E=-\varepsilon^2\quad \varepsilon>0\end{cases} \quad (20)$$

There is not the exact solution of the Schrödinger equation for most types of interaction. So, the kinds of various methods such as super symmetric method [22, 23] and Nikiforov-Uvarov method [18] have been used for the solution of this equation. As mentioned before, where:

$$\tilde{\tau} = D-1,\ \sigma = r,\ \sigma^2 = r^2,\ \tilde{\sigma} = -\varepsilon^2r^2 - \beta r - \gamma \quad (21)$$

Considering the NU method condition for $\pi(s)$ with some analysis and simplification, the following equation can be achieved:

$$\pi(r) = \frac{2-D}{2} \pm \frac{1}{2}(2\varepsilon r \pm \sqrt{(2-D)^2+4\gamma}) \quad (22)$$

And we have:

$$\tau = 1 - (2\varepsilon r - \sqrt{(2-D)^2+4\gamma}) \quad (23)$$

As mentioned before, we can use NU method to acquire the equation of energy. Therefore we have:

$$E = -\frac{2\mu}{\hbar^2}\frac{(2V_0\alpha+b\alpha)^2}{\left[2n+1+\sqrt{(2-D)^2+4(\frac{2\mu}{\hbar^2}(V_0+b)+l(l+D-2)}\right]^2} \quad (24)$$

having achieved this important equation, we can calculate the energy for ^6Li and ^7Li nuclei in their ground state by assigning appropriate values to coefficients of the potential. It is worth mentioning that in shell model, the nucleons are assumed as a two- also three particle system.

We have obtained the potential parameters by fitting the ground state of energy. In shell structure, the potential chosen parameters for ^6Li in which both n and l are set to 1, $V_0 = 80\ MeV$, $b = 100MeV$, $\alpha = 1.12\ fm^{-1}$ and for ^7Li $V_0 = 40MeV$, $b = 1MeV$, $\alpha = 0.00158fm^{-1}$.

And the wave functions of the quantum system are given by:

$$\psi = B_n r^{\frac{1}{2}((2-D)+\sqrt{(2-D)^2+4\gamma}} \times \exp(-\varepsilon r)L_n^{\sqrt{(2-D)^2+4\gamma}}(2\varepsilon r);$$

$$\gamma = \frac{2\mu}{\hbar^2}(V_0+b)+l(l+D-2) \quad (25)$$

Ground-state binding energies (E) for mentioned isotopes are summarized in Table1. We note that the two different ways used in this study are shell and cluster model. The results obtained from the cluster model are more consistent with the experimental results, although the difference between two models is very small.

Since the nucleus at the ground state have spin of $J^\pi = 1^+,\ 3/2^-$ then the effect of spin-orbit coupling on the L = 1 states cannot be ignored. Therefore, using Eq. (26), the effect of spin-orbit coupling on the energy levels is calculated as a first-order disturbing factor. The results of the calculation are shown in table1.

$$E_n^{(1)} = \langle n | V_{L.S}(r)\vec{L}.\vec{S} | n \rangle = \int \psi^*(r) \frac{\hbar^2}{2m_0^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \vec{L}.\vec{S}\psi(r) r^2 dr \quad (26)$$

TABLE 1. Ground-state binding energies (E) for Li isotopes in shell and cluster model and compared with experiment data and other results

Isotope	J^π	$E(MeV)$						
		Shell model	L.S	Cluster model	L.S	CDB_{2k} [2]	INOY [2]	Exp[24]
^6Li	1^+	31.6833	31.90	31.7296	31.8301	29.07(41)	32.33(19)	31.99
^7Li	$3/2^-$	39.6439	39.6857	39.1241	39.1741	35.56(23)	39.62(40)	39.24

Calculation of Electric Quadrupole Moment

The paired nucleons move in spherically symmetric orbits, they don't contribute to Q. therefore we might expect that for many nuclei, the quadrupole moment can be estimated from the valence nucleon, which we can assume to orbit near the surface. The electric quadrupole moment has been calculated for the qround state as [25]:

$$eQ = e\int \psi^*(3z^2 - r^2)\psi dv \quad (27)$$

From the above equation we understand that we need wave function of system to calculate electric quadrupole moment. The radial wave function is obtained from Eqs. (17) and (25), so we can easily calculate the electric quadrupole moment of studied isotopes by calculating Q in shell model and cluster model. In order to calculate the electric quadrupole moment, it is assumed that the wave function is concentrated in the xy-plane. For this reason, the quantity of quadrupole momentum is obtained negatively (see table2). The obtained results are shown in Table 2.

TABLE 2. Ground-state electric quadrupole moments (Q)

Isotope	$Q(eb)$					
	Shell model	Cluster model	CDB_{2k} [2]	INOY [2]	Exp[26]	value error
^6Li	-0.000823	-0.000813	-0.00066(40)	+0.00080(19)	-0.000806	0.0007232/ 0.000007
^7Li	-0.0413	-0.0406	-0.0320(22)	-0.0279(17)	-0.040	0.0013/0.0006

Finding the forces between the nucleons, the nuclei structure, and the nature of the nuclear interactions between them and also electric quadrupole, are considered as the main aims of studying nuclear physics. Good values obtained of the nuclear ground-state properties of the Li isotopes, such as the energy and electric quadrupole moments, are ideal tools for testing the validity of these nuclear models. These values are compared with predictions from shell-model and cluster-model calculations. Although the difference between them is too small but the electric quadrupole moment results in the cluster model are in good agreement with experimental results. Also the calculated energy and electric quadrupole moment in cluster model are close to the experimental data. Consequently, the suggested model can also be used for investigating other similar isotopes.

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