Volume 14, Number 4, 2021. pp. 333-338

Jordan Journal of Physics

ARTICLE

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

Jamshid K. Bizhaem, Nasrin Malekinezhad and **Mohammadreza Shojaei**

Department of Physics, Shahrood University of Technology, P.O. Box 36155-316, Shahrood, Iran.

Doi: **https://doi.org/10.47011/14.4.7**

Received on: 10/10/2020; *Accepted on: 01/12/2020*

Abstract: In this paper, we have investigated electric quadrupole moment of ^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 Schrödinger 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 compared the results obtained with experimental results. By having the wave function, we can obtain the quadrupole moment. These values are compared with predictions from shell-model and cluster-model calculations. Although the difference between them is small, 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 goals. The most important models in nuclear physics are shell and cluster models. Shell model is acceptable in nuclear physics and ^7Li and ^6Li are described in the shell model with p-shell wave functions. Cluster structure in nuclear physics 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. From the theoretical point of view, the energy of Li isotopes has been studied in many different ways [1, 4]. C. Forssen *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. Among different nuclear models, cluster model and shell model have considerable answers for

Corresponding Author: Jamshid K. Bizhaem **Email**: khosravi_1224@yahoo.com

nuclei, especially light nuclei. Since the wave function contains a lot of necessary information for descriptions of quantum system, solving equations such as Schrödinger equation in nonrelativistic quantum mechanics is very important [7]. The lithium isotopes have received much attention due to their 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 models, ground-state binding energies, wave functions and finally quadrupole moments of lithium isotopes by solving the non-relativistic equation (Schrödinger) 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, 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 Schrödinger 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 models describing many-particle systems in nuclear models. Studying the properties of many-particle systems is complex and difficult due to high degrees of freedom, so the cluster model is one of the useful solutions to solve this problem. Instead of investigating individual particles, we consider the interaction between clusters. According to the cluster model, the nuclei 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 defined. 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 predicting magic numbers. Evidence for the validity of the shell model comes from experimental observations, such as binding energy, spin … and so on.

Schrödinger Equation in Cluster Model

To investigate the nuclei, there are two perspectives: relativistic and non-relativistic, each of which is particularly important. In this work, we use a non-relativistic system. In non-relativistic quantum mechanics, the Schrödinger 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]:

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

The first step of studying the properties of nuclei in shell model and cluster model is choosing a suitable potential [14]. Due to 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 potentials having been studied by many researchers in physics and chemical physics [15, 16, 17]. In this work, we use inversely quadratic Yukawa (IQY) potential and due to nuclear force saturation at lower distances, we add a repulsive term potential as interaction between particles and clusters. V_0 is

the parameter describing the potential well depth, α represents the potential range and b is an adjustable parameter. By substituting 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 the 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]. the differential equation 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 transformation:

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

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 that $\tau(s)$ has a negative derivative. Additionally, λ is a parameter with the following definition:

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

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 the polynomial solutions of which 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 expressions into (8) and considering the NU method condition for $\pi(s)$ with some analysis and simplification, the following equation can be obtained:

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

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 Schrödinger equation as follows:

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

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

Schrödinger 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 consider 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 follows:

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

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 no exact solution of the Schrödinger equation for most types of interaction. So, 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:

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

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

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

And we have:

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

As mentioned before, we can use the 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- and 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 are: $V_0 = 80\ MeV,\ b = 100MeV,\ \alpha = 1.12\ fm^{-1}$ 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 the mentioned isotopes are summarized in Table1. We note that the two different ways used in this study are shell and cluster models. The results obtained from the cluster model are more consistent with the experimental results,

although the difference between the two models is very small.

Since the nuclei at the ground state have spin of $J^\pi = 1^+,\ 3/2^-$, 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.

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

TABLE 1. Ground-state binding energies (E) for Li isotopes in shell and cluster models 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 nucleons 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 the wave function of the system to calculate the electric quadrupole moment. The radial wave function is obtained from Eqs. (17) and (25), so we can easily calculate the electric quadrupole moment of the 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 Table 2). 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, the nature of the nuclear interactions between them and the electric quadrupole moment 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 energy and electric quadrupole moment, 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 very small, 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.

References

[1] Forssén, C., Caurier, E. and Navrátil, P., Phys. Rev. C, 79 (2009) 021303.

[2] Borremans, D. et al., Phys. Rev. C, 72 (2005) 044309.

[3] Neugart, R., Balabanski, D.L., Blaum, K., Borremans, D., Himpe, P., Kowalska, M., Lievens, P., Mallion, S., Neyens, G., Vermeulen, N. and Yordanov, D.T., Phys. Rev. Lett., 101 (2008) 132502.

[4] Roshanbakht, N. and Shojaei, M.R., Eur. Phys. J. A, 54 (2018) 134.

[5] Machleidt, R., Phys. Rev. C, 63 (2001) 024001.

[6] Doleschall, P., Phys. Rev. C, 69 (2004) 054001.

[7] Mousavi, M. and Shojaei, M. R., Adv. High-energy Phys., 2017 (2017) 5841701.

[8] Cederberg, J., Olson, D., Larson, J., Rakness, G., Jarausch, K., Schmidt, J., Borovsky, B., Larson, P. and Nelson, B., Phys. Rev. A, 57 (1998) 2539.

[9] Stone, N. J., Atomic Data and Nuclear Data Tables, 111–112 (2016) 1.

[10] Tanihata, I., Kobayashi, T., Yamakawa, O., Ekuni, K., Sugimoto, K., Takahashi, N., Shimoda, T. and Sato, H., Phys. Lett. B, 206 (4) (1988) 592.

[11] Beck, C., "Clusters in nuclei", Vols. 1, 2 & 3, (Springer-Verlag, Berlin, Heidelberg, 2010).

[12] Rajabi, A.A., Few-body Systems, 37 (2005) 197.

[13] Zoghi-Foumani, N., Shojae, M.R. and Rajabi, A.A., Pramana Journal of Phys., 88, (2017) 68.

[14] Binesh, Z., Shojaei, M.R. and Azadegan, B., Can. J. Phys., 98 (1) (2018) 28.

[15] Yukawa, H., Proc. Phys.-Math. Soc. Jpn., 17 (1935) 48.

[16] Rezvani, F. and Shojaei, M.R., U. P. B. Sci. Bull., Series A, 79 (2017) 3.

[17] Hamzavi, H., Ikhdair, S.M. and Ita, B.I., Physica Scripta, 85 (4) (2012) 045009.

[18] Nikiforov, A.F. and Uvarov, V.B., "Special Function of Mathematical Physics", (Birkhäuser Basel, 1988).

[19] Aslanzadeh, M. and Rajabi, A.A., Eur. Phys. J. A, 50 (2014) 1.

[20] Zhang, M.C., Sun, G.H. and Dong, S.H, Phys. Lett. A, 374 (2010) 704.

[21] Deta, U.A., Suparmi, A. and Cari, C., Adv. Studies Theor. Phys., 7 (2013) 647.

[22] Cooper, F., Khare, A. and Sukhatme, U., Phys. Rep., 251 (1995) 267.

[23] Feizi, H., Rajabi, A.A. and Shojaei, M.R., Acta Physica Polonica B, 42 (2011) 2143.

[24] Tilley, D.R., Cheves, C.M., Godwin, J.L., Hale, G.M., Hofmann, H.M., Kelley, J.H., Sheu, C.G. and Weller, H.R., Nucl. Phys. A, 708 (2002) 3.

[25] Krane, K.S., "Introductory Nuclear Physics", (John Wiley and Sons, Ltd., 1987).

[26] Stone, N.J., Atomic Data and Nuclear Data Tables, 90 (1) (2005) 75.