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Research Article

Two-Center Gaussian Potential Well for Studying Light Nucleus in Cluster Structure

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The clustering phenomena are very important to determine structure of light nuclei and deformation of spherical shape is inevitable. Hence, we calculated the energy levels of two-center Gaussian potential well including spin-orbit coupling by solving the Schrödinger equation in the cylindrical coordinates. This model can predict the spin and parity of the light nuclei that have two identical cluster structures.

1. Introduction

In the light nucleus, deformation plays an important role in determining nuclear structure. These deviations from spherical structures are found in the axial deformations and the clustering because numerous experimental studies have revealed clustering phenomena in them [1, 2]. Freer and Merchant in 1997 studied the role of clustering and cluster models in nuclear reactions and examined the evidence for α-cluster chain configurations in the even-even light nuclei from ^{8}Be to ^{28}Si [3, 4]. In 2001, Kanada-En'yo and Horiuchi showed that the valence neutrons in nucleus with cluster structure can form a covalent bond between the clusters and named it "nuclear molecules" [5]. For example, ^{9}Be has a neutron that exchanges between the two alpha clusters. They studied nuclear molecules by the one-center deformed harmonic oscillator potential [5, 6].

For studying light nucleus in cluster model, many physicists used various methods such as antisymmetrized molecular dynamics (AMD) [7] and fermionic molecular dynamics (FMD) [8] and condensates and the THSR Wave-Function [9–11]. These models have many important advantages for studying nuclei in cluster models but do not make assumptions about the cluster [12].

The two-center shell model is more appropriate for modeling nuclei with clustered nature. This model assumes a clustered structure, and each cluster is represented by its own potential. This potential is the two-center harmonic oscillator (TCHO) [13]. It has a complete analytical solution but does not have a sufficiently sharp edge to satisfy finite separation energies.

In this article, we consider axially symmetric nuclear parameterization, so the nuclear surface equation is given in the cylindrical coordinates [14, 15]. In this case, the deformation removes the degeneracy of single nucleon levels associated with spherical symmetry [16]. In the next section, we introduce new potential for studying the nucleus with the cluster structure.

2. 2D Potential in Cylindrical Coordinates

If the nucleus structure consists of two identical clusters, the nuclear surface in the cylindrical coordinates is defined by [15, 17]

$$\rho = \begin{cases} b\sqrt{1-\left(\dfrac{z+c_1}{a}\right)^2} & z \le z_1 \\ \rho_2 - \sqrt{R^2-(z-c_2)^2} & z_1 \prec z \prec z_2 \\ b\sqrt{1-\left(\dfrac{z-c_1}{a}\right)^2} & z_2 \le z, \end{cases} \qquad (1)$$

where $\pm c_1$ are the positions of the two cluster centers and other parameters are shown in Figure 1.

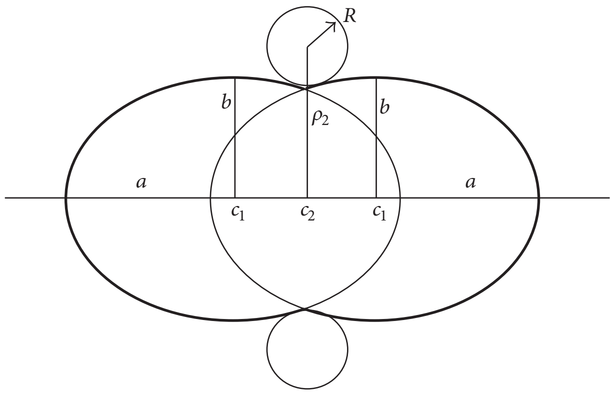


Figure 1: Parameterizations of nuclear shape in two cluster structures.

Hence, we use two-center Gaussian potential well for calculating the energy levels of nucleus which are nearly spherical or deformed because of having cluster structure. Our potential in cylindrical coordinates can be split into two parts:

$$V_0(\rho, z) = \begin{cases} A\exp\left(-\alpha(z-z_0)^2\right) + B\exp\left(-\beta\rho^2\right), & z \geq 0 \\ C\exp\left(-\lambda(z+z_0)^2\right) + B\exp\left(-\beta\rho^2\right), & z < 0, \end{cases} \quad (2)$$

where A, C, and B are the potential depth, the parameters α, β, and λ are inverse square range, and z_0 is cluster centers. We study nucleus that has two identical cluster structures. Hence, we suppose that the parameters $A = C$ and $\alpha = \lambda$ have a symmetric potential form. In Figure 2, the potential is plotted for some values of z_0. The nuclei with the closed shell such as ^{4}He nucleus have a spherical shape and are exceptionally stable. Hence, the spherical Gaussian potential well (Figure 2(a)) can describe energy levels of the nucleus that has a spherical shape. But in light nucleus with almost half full shells $N = 2$, the nucleons have been observed to cluster structure with a two-center structure. For example, ^{8}Be isotope at the ground state has two alpha cluster structures and decays to alpha particles by 92 keV energy. In this case, the potential in Figure 2(d) can be used to describe it. Likewise, for light neutron-rich nucleus that have covalent binding between two clusters due to valence neutrons, the potentials are shown in Figures 2(b) and 2(c).

If the potential of the quantum system to be examined is axially symmetric, then the Schrödinger equation in the cylindrical coordinates can be employed. For a three-dimensional problem, the Laplacian in cylindrical coordinates is used to express the Schrödinger equation in the following form:

$$\frac{-\hbar^2}{2M}\nabla^2\psi(\rho,\phi,z) + V_0(\rho,z)\psi(\rho,\phi,z) = E\psi(\rho,\phi,z), \quad (3)$$

where E and M denote the energy eigenvalue and the mass, respectively. $V_0(\rho, z)$ is potential that does not depend on ϕ because of the axial symmetry and is separable to $V_0(\rho)$ and $V_0(z)$. In the cylindrical coordinates, the Laplace operator takes the following form:

$$\nabla^2 = \frac{\partial^2\psi}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\psi}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2}. \quad (4)$$

The separation of variables is accomplished by substituting

$$\psi(\rho,\phi,z) = R(\rho)Z(z)\Phi(\phi). \quad (5)$$

In the usual way, this leads to the following ordinary differential equations [18]:

$$\frac{d^2\Phi(\phi)}{d\phi^2} + m^2\Phi(\phi) = 0, \quad (6)$$

$$\frac{d^2Z(z)}{dz^2} - \frac{2M}{\hbar^2}\left(V_0(z) - E\right)Z(z) + \gamma^2 Z(z) = 0, \quad (7)$$

$$\frac{d^2R(\rho)}{d\rho^2} + \frac{1}{\rho}\frac{dR(\rho)}{d\rho} - \left(\gamma^2 + \frac{m^2}{\rho^2}\right)R(\rho) - \frac{2M}{\hbar^2}V_0(\rho)R(\rho) = 0. \quad (8)$$

The solution of the first equation is

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}}\exp(im\phi), \quad (9)$$

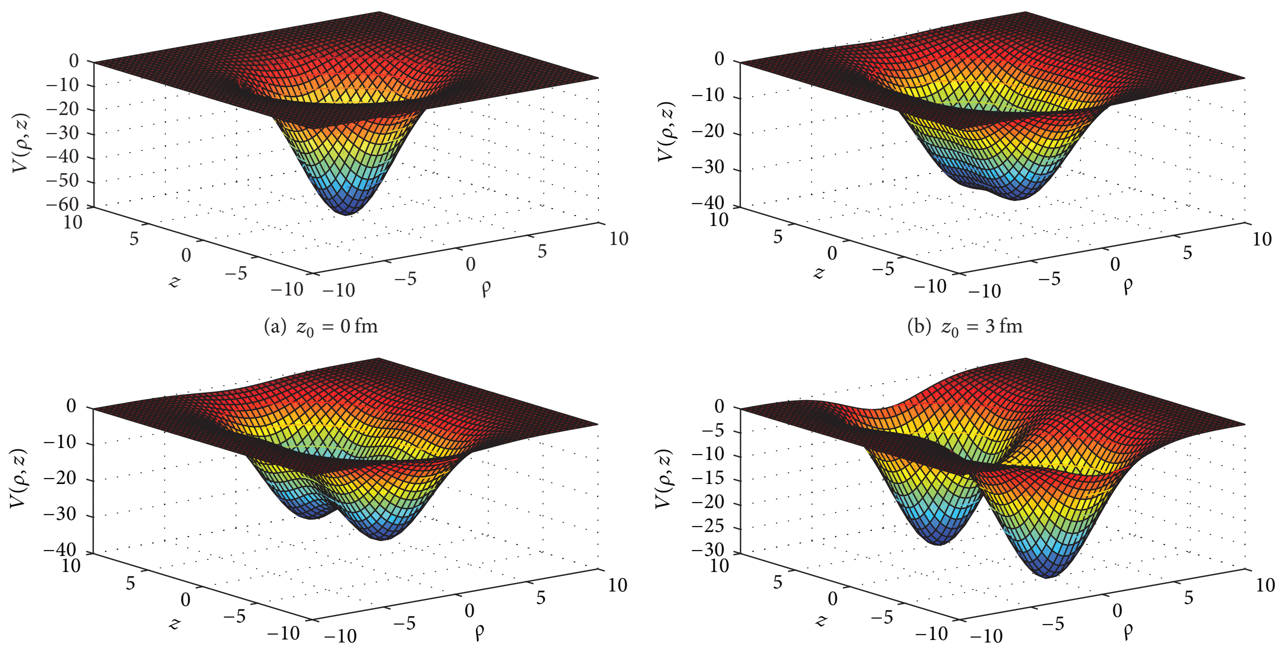
where m is the magnetic quantum number and integer. The next step is to obtain the solutions of (7) and (8) which cannot be solved by analytical methods. But the Hamiltonian is diagonal, and there are some numerical methods to solve it. We use a well-known Numerov's numerical method to solve ordinary differential equations of second order [19, 20]. In this method, we first organize the square matrix Hamiltonian of the system consisting of the kinetic energy matrix and the potential energy matrix; then we obtain the eigenvectors of Hamiltonian and the eigenvalues for the stationary states of the time-independent Schrödinger equation. The values of M and $\hbar$ are considered as $M = 1$ and $\hbar = 1$. The eigenvectors $R_{n_\rho}(\rho)$ for three lowest states are shown in Figure 3 and the eigenvectors $Z_{n_\nu}(z)$ are plotted for some values of z_0 in Figure 4. n_ρ is the radial quantum number and n_z is the quantum number along z-axis having values $0, 1, 2, \ldots$.

The eigenvectors $R_{n_\rho}(\rho)$ vanish on the boundaries of our system and behave as expected. For the eigenvectors $Z_{n_\nu}(z)$, in addition to boundary conditions, we consider the continuity conditions too:

$$\underset{z<0}{Z_{n_\nu}(z \longrightarrow 0)} = \underset{z>0,}{Z_{n_\nu}(z \longrightarrow 0)} \quad (10)$$

$$\underset{z<0}{\frac{\partial Z_{n_\nu}(z \longrightarrow 0)}{\partial z}} = \underset{z>0.}{\frac{\partial Z_{n_\nu}(z \longrightarrow 0)}{\partial z}} \quad (11)$$

While we describe nuclei in an axially symmetric model, the orbital angular momentum, l, and the intrinsic spin, s, are not



(a) $z_0 = 0$ fm (b) $z_0 = 3$ fm (c) $z_0 = 4$ fm (d) $z_0 = 5$ fm

Figure 2: The Gaussian potential for some values of z_0.

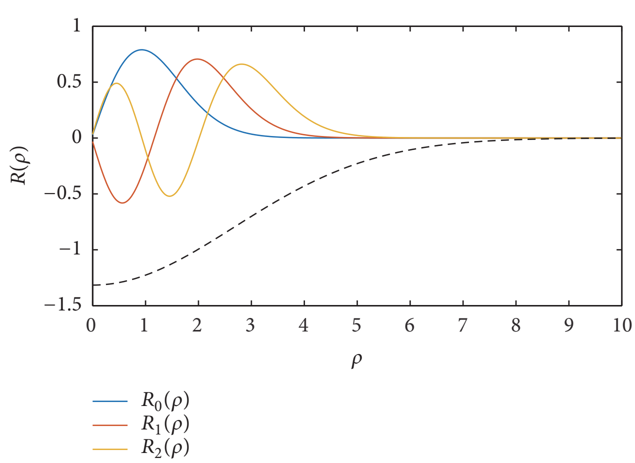


Figure 3: The eigenvectors $R_{n_\rho}(\rho)$ of three lowest states.

good quantum numbers because states with different l-values with the same parity can mix. In this model, the quantum number $N = n_\rho + n_z$ is the principal quantum number and the parity is determined by $(-1)^N$. The magnetic quantum number has the integer values between $-n_\rho$ and n_ρ too.

Figures 4(a)–4(d) show that the wave functions associated with z-axis have a definite parity with respect to $z = 0$. For finite separations, the wave functions do not feel the presence of the other cluster across the barrier in low energy. The energy levels with the same quantum number which located in the first or in the second potential well have the same value.

The eigenvalues from the solution of the Hamiltonian equation in z-axis are obtained for the different values of the distance between the two cluster centers, and the variation of them is given in Figure 5. In this figure, the shell structure of the spherical nucleus is reproduced for the two separate clusters, in higher energy. At $z_0 = 0$, there are the principal levels without spin-orbit coupling (N, m) and, for large values of z_0, the levels start to form two clusters and their levels overlap with each other.

One of the interesting features of Figure 5 is that states having the same z-component of angular momentum, m, repulse each other and prevent crossing. This is consistent with the theory of Neumann and Wigner. They showed that such level crossings are highly improbable [21].

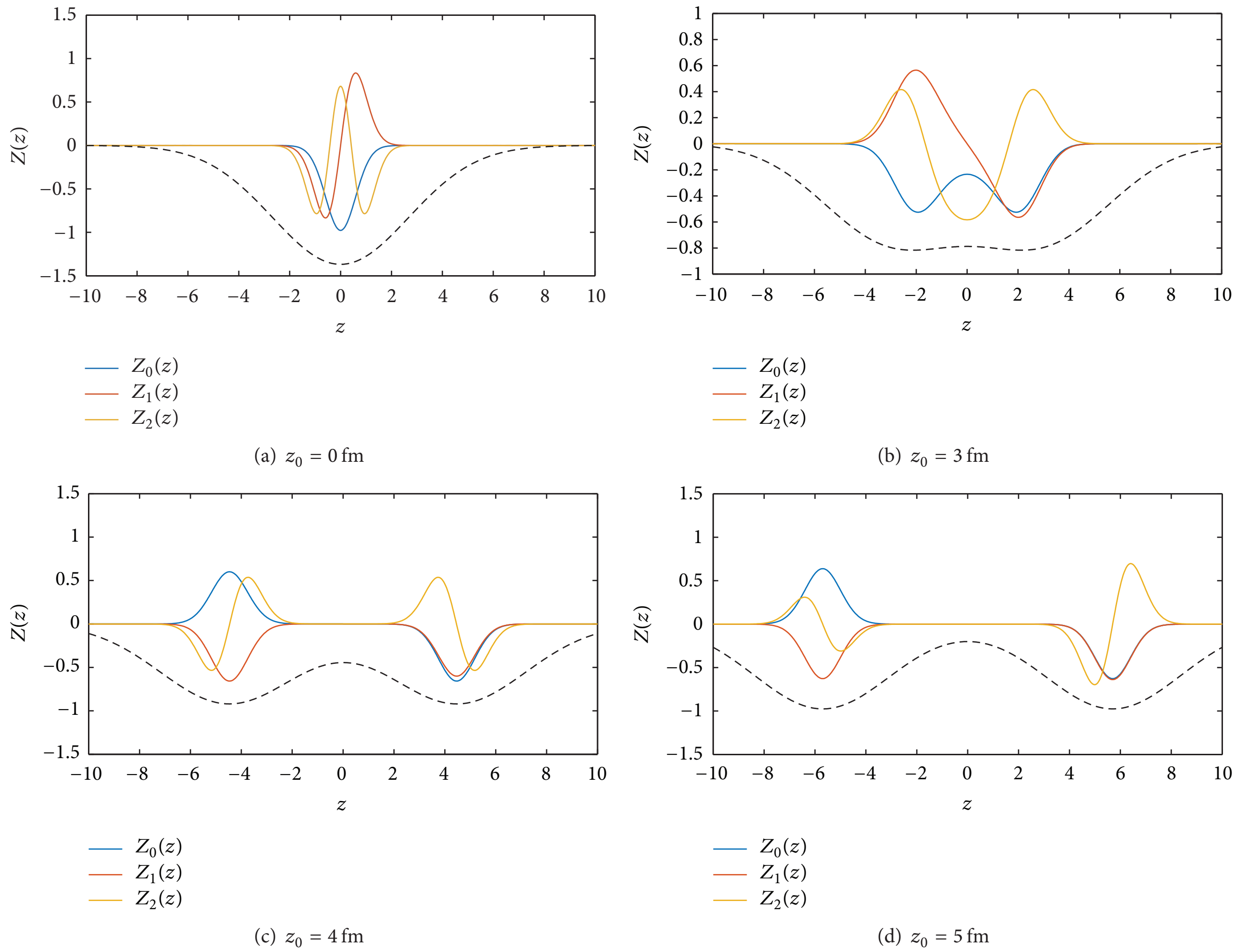
The levels with different values of n_ρ and n_z but the same value of N are degenerate. For example, $(n_z, n_\rho, m) = (1, 0, 0)$ are degenerate with $(n_z, n_\rho, m) = (0, 1, 0)$. We calculated the spin-orbit coupling to eliminate this degeneracy.

3. The Effect of Spin-Orbit Coupling on Levels

After the presentation of the solutions of the Schrödinger equation with the potential in (2), we want to explain the effect of spin-orbit coupling on the single particle levels for spherical nuclei and for nuclei with two cluster structures separated at an infinite distance.

The spin-orbit coupling is defined in the form of [15, 22]

$$V_{L\cdot S} = -\lambda \left(\frac{1}{2m_0 c}\right)^2 \vec{L}\cdot\vec{S}, \tag{12}$$



(a) $z_0 = 0$ fm

(b) $z_0 = 3$ fm

(c) $z_0 = 4$ fm

(d) $z_0 = 5$ fm

FIGURE 4: The eigenvectors $Z(z)$ of three lowest states for some values of z_0.

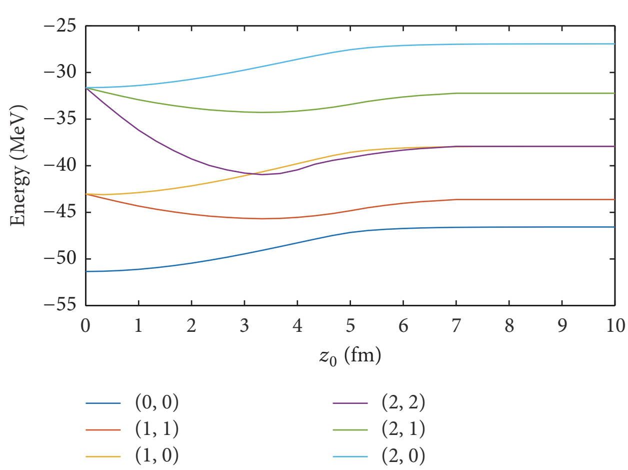


FIGURE 5: Variations of the eigenvalues in z-axis with the distance between the two cluster centers.

where $\lambda = 35$ is a dimensionless coupling constant; m_0 and c are the nucleon and the speed of the light, respectively [15].

The orbital angular momentum operator is $\vec{L} = \vec{\nabla} V \times \vec{p}$ and we must transform it into cylindrical coordinates:

$$\begin{aligned} \widehat{L}^{\pm} &= \mp\hbar e^{\pm i\varphi}\left(\frac{\partial V}{\partial \rho}\frac{\partial}{\partial z} - \frac{\partial V}{\partial z}\frac{\partial}{\partial \rho} \pm i\frac{\partial V}{\partial z}\frac{1}{\rho}\frac{\partial}{\partial \varphi}\right); \\ \widehat{L}_z &= i\hbar\frac{\partial V}{\partial \rho}\frac{1}{\rho}\frac{\partial}{\partial \varphi}, \end{aligned} \tag{13}$$

hence,

$$\vec{L}\cdot\vec{S} = \frac{1}{2}\left(L^{+}s^{-} + L^{-}s^{+}\right) + L_z s_z. \tag{14}$$

The shift of the energy levels due to the spin-orbit coupling was calculated using the orthogonality of the wave functions. The matrix elements of the spin operators are

$$\begin{aligned} \left\langle m_s' \left| \widehat{s}_+ \right| m_s \right\rangle &= \hbar\delta_{m_s', m_s+1}, \\ \left\langle m_s' \left| \widehat{s}_- \right| m_s \right\rangle &= \hbar\delta_{m_s', m_s-1}, \\ \left\langle m_s' \left| \widehat{s}_z \right| m_s \right\rangle &= \hbar m_s\delta_{m_s', m_s}, \end{aligned} \tag{15}$$

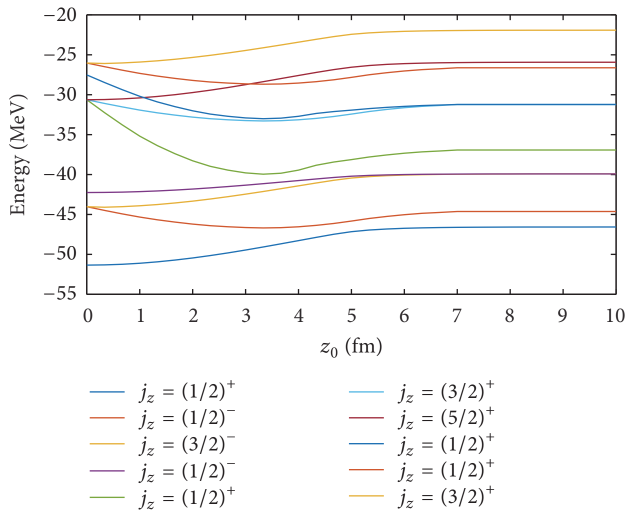


FIGURE 6: Variations of the eigenvalues (n_z, n_ρ, m) in z-axis including spin-orbit coupling with the distance between the two cluster centers.

and the spin-orbit matrix is

$$\begin{aligned} &\left\langle n'_z, n'_\rho, m', m'_s \left| \frac{1}{2}\left(L^+ s^- + L^- s^+\right) + L_z s_z \right| n_z, n_\rho, m, m_s \right\rangle \\ &= \frac{\hbar}{2} \left\langle n'_z, n'_\rho, m' \left| L^+ \right| n_z, n_\rho, m \right\rangle \delta_{m'_s, m_{s-1}} \\ &+ \frac{\hbar}{2} \left\langle n'_z, n'_\rho, m' \left| L^- \right| n_z, n_\rho, m \right\rangle \delta_{m'_s, m_{s+1}} \\ &+ \hbar m_s \left\langle n'_z, n'_\rho, m' \left| L_z \right| n_z, n_\rho, m \right\rangle \delta_{m'_s, m_s}. \end{aligned} \tag{16}$$

Now, we use the parabolic approximation [23], and consequently the levels of single particle energies are obtained as a function of z_0 by the diagonalization of the potential $V_0 + V_{L\cdot S}$. The structure of levels is plotted in Figure 6 and labeled them by j_z. In our model, the projection of the total angular momentum on the symmetry axis, $j_z = m + m_s$, is the good quantum number. Hence, states of different j_z are not coupled by the Hamiltonian but the states with $\pm j_z$ are degenerate because the nuclei have reflection symmetry for either of the two possible directions of the symmetry axis.

In Figure 6, the level scheme of the spherical nuclei is obtained for $z_0 = 0$. But, by increasing z_0, two separated clusters are formed. An example of light nuclei by two cluster structures is ^{9}Be isotope. The nucleon single particle level scheme is plotted in Figure 6. ^{9}Be isotope is stable and has 4 protons and 5 neutrons. Alpha cluster is in the first level and in the second level there will be other alpha clusters and the remaining single nucleon located in the next level. Experimental evidence for ^{9}Be shows that it has a ground state with spin and parity $3/2^-$ and a $1/2^+$ excited state [24, 25]. For predicting these results, we must use the potential well in Figure 4(b). When two separate centers in potential well are formed, the levels $(1, 0, 0)$ and $(0, 1, 0)$ overlap with each other. In our model, the single neutron is in the level $J_z = 3/2$ at the ground state and its parity is $(-1)^N = -1$. For the first excited state, the single neutron moves into level $J_z = 1/2^+$. We will predict other excited states by considering the rotational band and Coulomb potential between the clusters.

4. Conclusion

In light nuclei, close to decay threshold, the cluster phenomenon is the favored mode. Hence, we use two-center Gaussian potential well for calculating the energy levels of nucleus which are nearly spherical or deformed because of having two identical cluster structures. We solved the Schrödinger equation in the cylindrical coordinates and plotted the level scheme without considering spin-orbit coupling. Then we modified results with it. For $z_0 = 0$, the level scheme of the spherical nuclei is obtained, and two separated clusters are formed by increasing z_0. In principle, a two-center potential well can be used to study light nuclei with two cluster structures and make assumptions about the cluster in them.

Competing Interests

The authors declare that they have no competing interests.

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