Cluster Structure in Be Isotopes within Point-Coupling Covariant Density Functional 

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The potential energy surfaces and density distributions of ground states in even-mass Be isotopes are studied by using the point-coupling covariant density functional theory with the PC-F1 effective interaction. The clustering structure is exhibited automatically in most of the Be isotopes. The results indicate that the Be clustering structure, while pronounced in even-mass Be nuclei, is only noticeable in 6Be. However, the α-cluster structure is in-beam investigated in 6Be. The point-coupling CDFT has recently attracted more and more attention due to its advantages and potential applications. In this work, the ground-state properties of even-mass Be isotopes are investigated by analyzing the potential energy surfaces (PES), density distributions and single-particle energy levels.

In the CDFT with point-coupling interaction, the energy density functional is written as

\[ E_{\text{EDF}} = \sum_k \int dr \bar{\psi}_k \gamma_i (\mathbf{r}) (-i \gamma \cdot \nabla + m) \psi_k (\mathbf{r}) \]

\[ + \int dr \left( \frac{\alpha_s}{2} \rho_s^2 + \frac{\beta_s}{3} \rho_s^3 + \frac{\gamma_s}{4} \rho_s^4 + \frac{\delta_s}{2} \rho_s \Delta \rho_s \right) \]

\[ + \frac{1}{2} \alpha_{\nu} \mu \Delta \mu + \frac{1}{4} \gamma_{\nu} \mu \Delta \mu^2 + \frac{1}{4} \Delta \rho_s \]

\[ + \frac{1}{2} \alpha_{\nu} \mu \Delta \mu + \frac{1}{4} \gamma_{\nu} \mu \Delta \mu^2 + \frac{1}{4} \Delta \rho_s \]

\[ + \frac{1}{4} F_{\mu \nu} F^{\mu \nu} - F_{0 \mu} \partial_0 A_\mu + e \left( 1 - \frac{\gamma_{\nu} \mu \Delta \mu}{2} \right) \]

\[ \psi_k (\mathbf{r}) \text{ is the nucleon Dirac spinor field, } m \text{ is the nucleon mass, and } e \text{ is the charge unit for protons.} \]

\[ \text{There are nine coupling constants } \alpha_s, \alpha_{\nu}, \alpha_{\nu}, \alpha_{\mu}, \alpha_{\mu}, \alpha_{\nu}, \alpha_{\nu}, \alpha_{\mu}, \alpha_{\mu}. \]

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The quadrupole deformation parameter $\beta$ is related to $\langle Q_2 \rangle$ by $\langle Q_2 \rangle = \frac{3}{5R_A^2}A \beta R$, $A$ is the mass number and $R = r_0 A^{1/3}$ ($r_0 = 1.2$) fm. Here $C$ is the corresponding curvature constant and $q_2$ is the constrained value of the quadrupole moment.\cite{45}

In the calculation, we use a popular parameterized relativistic functional PC-F1\cite{44} for the particle-hole channel. The solution of the equation of motion for the nucleons is accomplished by an expansion of the Dirac spinors in a set of three-dimensional harmonic oscillator basis functions in Cartesian coordinates with 14 major shells. The intrinsic triaxially deformed states are obtained as solutions of the self-consistent relativistic mean-field (RMF) equations constrained on the mass quadrupole moment related to the parameter $\beta$ varying $\beta \in [-1.5, 2.0]$ with step size $\Delta \beta = 0.1$. We choose $z$ axis as the symmetry axis, the density distributions are plotted in the $zx$ plane.

![Fig. 1.](image)

Figure 1 shows the PES of even-mass Be isotopes as a function of the axial deformation parameter $\beta$ obtained by the constrained CDFT calculations using the PC-F1 set for even-mass $^6$–$^{14}$Be.

The total binding energies, single-nucleon wave functions, and other Observables are generated from self-consistent solutions of the above equations. For lighter nuclei, the density distributions are insensitive to pairing correlations.\cite{45} Therefore, the pairing correlations are not taken into account in our results.

Unrestricted CDFT calculation gives only a local minimum on the PES. The total energies of different deformations are obtained by imposing a quadratic constraint on the mass quadrupole moment

$$\langle H \rangle + \frac{1}{2}C(\langle \hat{Q}_2 \rangle - q_2)^2,$$

where $\langle H \rangle$ is the total energy, and the mass quadrupole operator $\hat{Q}_2$ reads

$$\hat{Q}_2 = 2z^2 - x^2 - y^2.$$  

In Table 1, we present the properties for the ground state of even-mass $^6$–$^{14}$Be from the CDFT calcula-
utions with PC-F1 effective interaction, including the calculated binding energies, quadrupole deformation parameters and the corresponding root-mean-square (rms) radii. The experimental binding energies\(^{[17]}\) of even-mass Be isotopes are well reproduced except \(^{8}\text{Be}\). In particular, the calculated binding energy of \(^{12}\text{Be}\) is exactly consistent with the calculation of density-dependent relativistic mean-field theory\(^{[48]}\). Moreover, it is noted that the quadrupole deformation parameters of nuclei are changing with neutron number. Starting from a prolate deformed shape with \(\beta = 0.86\) in \(^{6}\text{Be}\), the deformation is maximum in \(^{8}\text{Be}\), and then continually decreases down to zero in \(^{12}\text{Be}\). With two neutrons more than \(N = 8\), the ground state becomes prolate deformed again in \(^{14}\text{Be}\), as shown in Fig. 1. It is known that the rms radius indicates the spatial distribution of the atomic nucleus. As is expected, \(^{12}\text{Be}\) has the smallest proton rms radius due to shell closure at \(N = 8\). In the neutron drip line region, there is the largest difference between the neutron rms radius and the proton rms radius for \(^{14}\text{Be}\).

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Theor. BE (MeV)</th>
<th>Expt. BE (MeV)</th>
<th>(\alpha)</th>
<th>(\beta)</th>
<th>Total BE (MeV)</th>
<th>Neutron (R_{\text{rms}}) (fm)</th>
<th>Proton (R_{\text{rms}}) (fm)</th>
<th>Total (R_{\text{rms}}) (fm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{8}\text{Be})</td>
<td>-24.349</td>
<td>-26.923</td>
<td>0.26</td>
<td>1.16</td>
<td>0.86</td>
<td>2.037</td>
<td>2.731</td>
<td>2.521</td>
</tr>
<tr>
<td>(^{10}\text{Be})</td>
<td>-47.368</td>
<td>-56.499</td>
<td>1.27</td>
<td>1.29</td>
<td>1.28</td>
<td>2.574</td>
<td>2.594</td>
<td>2.584</td>
</tr>
<tr>
<td>(^{12}\text{Be})</td>
<td>-61.025</td>
<td>-64.976</td>
<td>0.41</td>
<td>0.66</td>
<td>0.51</td>
<td>2.566</td>
<td>2.364</td>
<td>2.487</td>
</tr>
<tr>
<td>(^{14}\text{Be})</td>
<td>-70.832</td>
<td>-68.649</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>2.768</td>
<td>2.344</td>
<td>2.634</td>
</tr>
</tbody>
</table>

\(\rho_n\) \(\rho_p\) \(\rho\) \(\beta = 0.86\)

\(\rho_n\) \(\rho_p\) \(\rho\) \(\beta = 1.28\)

\(\rho_n\) \(\rho_p\) \(\rho\) \(\beta = 0.51\)

\(\rho_n\) \(\rho_p\) \(\rho\) \(\beta = 0.00\)

\(\rho_n\) \(\rho_p\) \(\rho\) \(\beta = 0.86\)

Figure 2 displays the density distributions of neutrons, protons and matter from the CDFT calculations using the PC-F1 set for the even-mass isotopes of Be.

Fig. 2. (Color online) The density distributions of neutrons, protons and matter from the CDFT calculations using the PC-F1 set for the even-mass isotopes of Be.

Table 1. The calculated binding energies (BEs), quadrupole deformation parameters (\(\beta\)) and the corresponding rms radii (\(R_{\text{rms}}\)) for the even-mass isotopes of Be obtained by PC-F1, compared with the experimental data available.

With the increase of neutron number, the distances undergo a decrease first and then increase, which is in agreement with the AMD calculations.\(^{[8]}\) With the increase of neutron number, a dramatic change in the density distributions of neutrons is observed. The density distributions of protons change with those of neutrons.

The clustering structure can be understood from the distributions of single-particle levels. Taking \(^{8,14}\text{Be}\) as examples, in Fig. 3, we plot the single-particle energies of neutrons and protons versus the axial deformation parameter \(\beta\). The dotted curves denote the corresponding Fermi surface. The solid line represents even parity level, while the dashed line stands for odd parity level. \(^{8}\text{Be}\) has the same configurations of \((1s_1/2)^2(1p_3/2)^2\) for protons and neutrons. The corresponding configurations of \(^{14}\text{Be}\) are \((1s_1/2)^2(1p_3/2)^2\) for protons and...
and \((1s_{1/2})^2(1p_{3/2})^4(1p_{1/2})^2(2s_{1/2})^2\) for neutrons. A lower-than-average density of single-particle levels around the Fermi energy results in extra binding from shell correction, whereas a larger-than-average value reduces binding. The density of single-particle levels near the Fermi surface in the oblate side is much larger than that in the prolate side. Therefore, large energy gaps around the Fermi surface in the single-particle levels often correspond to the minima on the PES.

![Graph](image)

**Fig. 3.** (Color online) Single-particle energies of (left panels) neutrons and (right panels) protons in \(^{8,14}\)Be versus the quadrupole deformation parameter \(\beta\). The dotted curves denote the corresponding Fermi surface.

In summary, we have studied the \(\alpha\)-cluster structure in the ground state of even-mass Be isotopes within the framework of the CDFT with the PC-F1 effective interaction. Our calculated binding energies agree well with the experimental values except \(^8\)Be. The calculated results show that \(^{12}\)Be is a spherical nucleus, and other nuclei are prolate deformed. Moreover, the \(\alpha-\alpha\) distances and the corresponding quadrupole deformation parameters have a similar evolution trend against the neutron number. It is suggested that \(^6\)Be has an \(\alpha+2p\) clustering structure, while even-mass \(^{8,10,14}\)Be have \(2\alpha\) clustering structure. As the number of neutrons increases, the density distributions of protons change in a similar way as those of neutrons.

It has to be pointed out that most of the Be isotopes are soft under the distortion of shapes. The beyond mean-field effects may have an influence on the density distributions. It will be very interesting to analyze this effect on the cluster in the future.

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