Deformation Effect on the Center-of-Mass Correction Energy in Nuclei Ranging from Oxygen to Calcium *

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The microscopic c.m. correction energies for nuclei ranging from oxygen to calcium are systematically calculated by both spherical and axially deformed relativistic mean-field (RMF) models with the effective interaction PK1. The microscopic c.m. correction energies strongly depend on the isospin as well as deformation and deviate from the phenomenological ones. The deformation effect is discussed in detail by comparing the deformed with the spherical RMF calculation. It is found that the direct and exchange terms of the c.m. correction energies are strongly correlated with the density distribution of nuclei and are suppressed in the deformed case.

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The mean field approximation is one of the most successful theoretical approaches in quantitatively describing the properties of both nuclear matter and finite nuclei near or far from the stability line. However, for a finite nuclear system, the translational symmetry of ground-state wave function is violated due to the localization of the center-of-mass (c.m.) in the mean field potential. In comparison with the preservation of rotational symmetry for the spherical nuclei and/or particle-number symmetry for the closed shell nuclei, the translational symmetry violation, probably as the most important case of symmetry breaking, is compulsory for all the nuclei. Therefore, it is necessary to develop proper methods for the translational symmetry restoration.

A rigorous way to restore the broken translational symmetry is the projection method, namely, projecting the ground-state wave function onto a good c.m. momentum. In principle, variation-after-projection (VAP)^[1] is an ideal solution in comparison with projection-after-variation (PAV) since it restores full Galilean invariance.^[2] However, it is numerically too expensive and impractical to be used in large-scale investigations. Hence, PAV is often used as a simpler treatment to give the c.m. correction energy. For the sake of feasibility and transferability, a standard way, i.e., expanding the correction in orders of the total momentum in c.m. frame $\langle P_{
m c.m.}^{2n}
angle$ and stopping at first order, is suggested, which is denoted as the microscopic c.m. correction method.^[3] In addition, phenomenological c.m. correction is also widely used in practical applications.^[4,5] It has been shown that the c.m. correction gives a remarkable contribution to the total binding energy in light nuclei (e.g., about 9% in 16 O).^[6]

mean field theory, the relativistic mean-field (RMF) theory^[7] has received a great deal of attention during the past decades.^[8,9] In RMF theory, both the phenomenological and microscopic c.m. correction are adopted to give the c.m. correction energy. Therefore, it is interesting to investigate the differences between these two c.m. correction methods. Since the microscopic c.m. correction energy is decided by the ground-state wave function, it is expected that it depends not only on the mass number, but also on the deformation of the nuclei. While in the phenomenological case, the deformation effect usually does not account for the c.m. correction energy. So far, a systematic study of the deformation effect on the microscopic c.m. correction energy in a large-scale nuclear mass region has not been given.

In this Letter, the microscopic c.m. correction energies for nuclei ranging from oxygen to calcium are investigated systematically in the spherical and axially deformed RMF models, and compared with the phenomenological ones. Furthermore, the deformation effects on the c.m. correction energies are studied in detail.

The starting point of the RMF theory is an effective Lagrangian density where nucleons are described as Dirac spinors ψ which interact via the exchange of several mesons (the isoscalar scalar σ , the isoscalar vector ω , and isovector vector ρ) and the photon.^[8,9] The detailed formulation of the RMF theory can be found in Refs. [8,9].

The microscopic c.m. correction energy is given by

$$E_{\rm c.m.}^{\rm mic} = -\frac{1}{2MA} \langle \boldsymbol{P}_{\rm c.m.}^2 \rangle, \qquad (1)$$

where $P_{\text{c.m.}} = \sum_{i}^{A} p_{i}$, which is given by the sum of the single-particle momentum operators p_{i} , is the to-

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tal momentum operator in the c.m. frame. The expectation value of $P_{\rm c.m.}^2$ is

$$\langle \boldsymbol{P}_{\text{c.m.}}^2 \rangle = \sum_a p_{aa}^2 - \sum_{a,b} \boldsymbol{p}_{ab} \cdot \boldsymbol{p}_{ab}^*, \qquad (2)$$

where a and b denote the occupied single-particle states. The expectation value of p_i^2 in the state $|a\rangle$ is denoted as p_{aa}^2 , and p_{ab} is the off-diagonal singleparticle matrix element between the state $|a\rangle$ and $|b\rangle$. Therefore, the correction energy in Eq. (1) can be decomposed into the direct term $E_{\rm c.m.}^{\rm dir}$ and the exchange term $E_{\rm c.m.}^{\rm exc}$,

$$E_{\rm c.m.}^{\rm dir} = -\frac{1}{2MA} \sum_{a} p_{aa}^2,$$
 (3a)

$$E_{\rm c.m.}^{\rm exc} = \frac{1}{2MA} \sum_{a,b} \boldsymbol{p}_{ab} \cdot \boldsymbol{p}_{ab}^*.$$
(3b)

It shows that $E_{c.m.}^{dir}$ increases while $E_{c.m.}^{exc}$ decreases the binding energy of a given nuclei. The further evaluations of Eq. (2) in spherical and axially symmetry are outlined in Ref. [3].

As the microscopic calculation of $E_{\text{c.m.}}^{\text{mic}}$ in Eq. (1) is often very time consuming, several phenomenological approaches are proposed, including the phenomenological formulas from harmonic oscillator states,

$$E_{\rm c.m.}^{\rm osc} = -\frac{3}{4} 41 A^{-1/3} \text{ MeV},$$
 (4)

and a fit to the microscopic c.m. correction energies calculated with the Skyrme interaction Z_{σ} ,^[5]

$$E_{\rm c.m.}^{\rm fit} = -17.2A^{-0.2}$$
 MeV. (5)

In the present work, the microscopic c.m. correction energies for nuclei with $8 \leq Z \leq 20$ are calculated in both the spherical and axially deformed RMF theory with the non-linear effective interaction PK1.^[6] In the calculation, the time-odd component for odd-Aand odd-odd nuclei^[10] is not included as its influence on the c.m. correction energy is negligible.^[11] The Dirac equation for nucleons and the Klein–Gordon equations for mesons are solved using the expansion method with the harmonic-oscillator basis.^[12] In the following investigation, 14 shells are used for both the fermion fields and the meson fields. As the microscopic c.m. correction energies are the main concern here, the pairing correlations are not included.

The microscopic c.m. correction energies $E_{\rm c.m.}^{\rm mic}$ of the nuclei ranging from oxygen to calcium calculated in the spherical and axially deformed RMF theory are shown in Fig. 1 as functions of the mass number Aand compared with the phenomenological $E_{\rm c.m.}^{\rm osc}$ and $E_{\rm c.m.}^{\rm fit}$. It is found that both the microscopic and phenomenological c.m. correction energies increase with the mass number systematically. $E_{\rm c.m.}^{\rm fit}$ is always larger than $E_{\rm o.m.}^{\rm osc}$ in this mass region, and the microscopic c.m. correction energies of most nuclei are in between with strong isospin dependence. Generally speaking, $E_{\text{c.m.}}^{\text{fit}}$ is more suitable for neutron-rich nuclei, whereas $E_{\text{c.m.}}^{\text{soc}}$ for nuclei around N = Z.



Fig. 1. Microscopic c.m. correction energies $E_{\text{c.m.}}^{\text{mic}}$ (solid lines) of nuclei with $8 \leq Z \leq 20$ in the spherical (a) and axially deformed (b) RMF calculations with the effective interaction PK1, in comparison with two phenomenological results $E_{\text{c.m.}}^{\text{osc}}$ and $E_{\text{c.m.}}^{\text{fit}}$ (dashed lines). The solid lines from the left to the right respectively correspond to the isotopic chains from oxygen to calcium.

From Fig. 1, the deformation effects on the microscopic c.m. correction energies are revealed by comparing the spherical and deformed results. Such deformation effects are extracted from the differences of microscopic c.m. correction energies between deformed RMF calculations $E_{\rm c.m.}^{\rm def}$ and spherical ones $E_{\rm c.m.}^{\rm sph}$, i.e., $\Delta E_{\rm c.m.} = E_{\rm c.m.}^{\rm def} - E_{\rm c.m.}^{\rm sph}$, and illustrated in Fig. 2(a) as a function of the quadrupole deformation parameter β obtained in the deformed RMF calculations. For $|\beta| < 0.1$, $\Delta E_{\rm c.m.}$ almost vanishes. While for $|\beta| > 0.1$, most of the $|\Delta E_{\rm c.m.}|$ increase with $|\beta|$ upto about 0.5 MeV.

In order to understand the non-unilateral effect of deformation on the microscopic c.m. correction energies, the direct $E_{\rm c.m.}^{\rm dir}$ and exchange term $E_{\rm c.m.}^{\rm exc}$ in Eqs. (3a) and (3b) are calculated, respectively. Their corresponding differences $\Delta E_{\rm c.m.}^{\rm dir}$ and $\Delta E_{\rm c.m.}^{\rm exc}$ between the deformed and spherical calculations are shown in Fig. 2(b) as functions of the quadrupole deformation parameter β . Different from $\Delta E_{\text{c.m.}}$, it is found that both $\Delta E_{\text{c.m.}}^{\text{dir}}$ and $\Delta E_{\text{c.m.}}^{\text{exc}}$ vary monotonously with $|\beta|$. Due to the different signs in $E_{\rm c.m.}^{\rm dir}$ and $E_{\rm c.m.}^{\rm exc}$, $\Delta E_{\rm c.m.}^{\rm dir}$ increases with deformation up to 1 MeV and $\Delta E_{\rm c.m.}^{\rm exc}$ decreases with deformation down to -0.6 MeV. Therefore, for a given nucleus, both spherical $|E_{c.m.}^{dir}|$ and $|E_{\rm c.m.}^{\rm exc}|$ are found to be larger than their corresponding deformed ones and the non-unilateral effect of deformation on the microscopic c.m. correction energies is just due to the competition between $E_{\rm c.m.}^{\rm dir}$ and $E_{\rm c.m.}^{\rm exc}$.



Fig. 2. Differences of the microscopic c.m. correction energy $\Delta E_{\rm c.m.} = E_{\rm c.m.}^{\rm def} - E_{\rm c.m.}^{\rm sph}$ (a) and their corresponding direct term $\Delta E_{\rm c.m.}^{\rm dir}$ (open circles) and exchange term $\Delta E_{\rm c.m.}^{\rm exc}$ (filled squares) (b) between deformed RMF calculations $E_{\rm c.m.}^{\rm def}$ and the corresponding spherical ones $E_{\rm c.m.}^{\rm sph}$ for nuclei with $8 \leq Z \leq 20$ as functions of the deformation parameter β .



Fig. 3. Differences of the matter rms radii ($\Delta R = R_{\rm def} - R_{\rm sph}$) between axially deformed RMF calculations $R_{\rm def}$ and the corresponding spherical ones $R_{\rm sph}$ for nuclei with $8 \leq Z \leq 20$ as a function of the deformation parameter β .

Since the matter rms radii as well as the microscopic c.m. correction energies are measures for the localization of the many-body wave function, it is interesting to investigate their correlations. Figure 3 shows the differences of the matter rms radii (i.e.,
$$\begin{split} \Delta R &= R_{\rm def} - R_{\rm sph} \end{split} \text{between } R_{\rm def} \text{ given by axially deformed RMF calculations and } R_{\rm sph} \text{ by spherical ones} \\ \text{as a function of the quadrupole deformation parameter} \\ \beta. It is clear that ΔR increases monotonously up to the maximum of (~ 0.1 fm) with <math>|\beta|$$
, and exhibits a similar behavior as $\Delta E_{\rm c.m.}^{\rm din}$ and $|\Delta E_{\rm c.m.}^{\rm exc.}|$ shown in Fig. 2(b). In addition, $R_{\rm def}$ is always larger than $R_{\rm sph}$. As a larger radius corresponds to smaller p_{aa}^2 and $p_{ab} \cdot p_{ab}^*$ in Eqs. (3a) and (3b), it leads to a suppression on both the direct and exchange term of $E_{\rm c.m.}^{\rm mic}$ in the deformed RMF calculations. Therefore, the direct term and exchange term of $E_{\rm c.m.}^{\rm mic}$ serve also as measures for the density distribution of nuclei.

In summary, a systematic study of the microscopic c.m. correction energies for nuclei with 8 \leq Z < 20 has been performed by the spherical and deformed RMF models with the effective interaction PK1. The microscopic c.m. correction energies, which are found between the phenomenological $E_{\rm c.m.}^{\rm fit}$ and $E_{\rm c.m.}^{\rm osc}$, strongly depend on the isospin as well as the deformation of the nuclei. The deformation effect on $E_{\rm c.m.}^{\rm mic}$ is clarified by comparing the deformed and spherical RMF calculations. In comparison with the spherical calculations, a suppression on both the direct and exchange terms of $E_{\text{c.m.}}^{\text{mic}}$, which even reach 1 MeV for the former and 0.6 MeV for the latter, is found in the deformed case. Moreover, it is illustrated that the direct and exchange terms of the c.m. correction energies are correlated with the density distribution of nuclei.

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