Center-of-mass correction and rotational correction in covariant density functional theory *

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Abstract: Center-of-mass (c.m.) correction and rotational correction in even-even Ge isotopes are systematically investigated within the triaxially deformed relativistic Hartree-Bogoliubov model using the PC-PK1 force. The shell effect and deformation effect on the microscopic c.m. correction and rotational correction are discussed, and the importance of both corrections on reproducing the binding energy is demonstrated.

Key words: center-of-mass correction, rotational correction, even-even Ge isotopes, covariant density functional theory

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1 Introduction

Nuclear energy density functional theory (DFT) plays a significant role in the microscopic and universal description of nuclei and has been the most promising tool for the global investigation of the properties of nuclei [1].

During the past few decades, covariant density functional theory (CDFT) has received widespread attention due to its great successes in the description of many nuclear phenomena [2–4]. There exist a number of attractive features in CDFT, especially in its practical applications in the self-consistent relativistic mean-field framework [2–4]. It gives naturally the spin-orbit potential. The relativistic effects are responsible for the pseudospin symmetry [5–8] in the nuclear single-particle spectra. Moreover, it is of particular importance that CDFT includes a consistent description of currents and time-odd fields which play important roles in the nuclear rotations [9–12].

In the framework of the CDFT, the relativistic Hartree-Bogoliubov (RHB) model [2] has been established by treating the mean-field and pairing correlation in a unified and self-consistent way and applied to the quantitative description of open-shell nuclei. In most RHB applications, the Gogny force [13] or the zero-range δ force [14] is employed in the pairing part. Recently, the separable pairing force [15] has attracted more and more attention due to its simplicity and reliability. Moreover, the triaxially deformed RHB (3DRHB) model with this separable pairing force has been developed in Ref. [16], which allows calculations for nuclei with triaxial shapes.

As a mean-field approach, however, the RHB model violates the translational symmetry of the ground-state wave function due to the localization of the center-of-mass (c.m.) in the mean-field potential. Of course, the restoration of this broken symmetry will introduce more correlation in the energy density functional and make the nucleus more binding. Therefore, the c.m. correction energy is usually considered in the RHB calculation either in a microscopic [17] or in a phenomenological [18, 19] way.

Moreover, for a deformed nucleus, the rotational symmetry is further violated in the RHB model and thus the corresponding rotational correction energy should also be considered. On one hand, the rotational symmetry, in principle, can be restored with the sophisticated angular momentum projection method [20]. However, this method can hardly be applied to systematical investigations because of the numerical complexity. On the other hand, the rotational correction can be approximately calculated in a much more economic way by using the cranking approximation [21].

In this paper, both the c.m. correction and the rotational correction are systematically investigated within the 3DRHB model by taking even-even Ge isotopes as

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examples, which present a rich shape structure, including spherical, prolate, oblate, and triaxially deformed shapes.

2 Theoretical framework

The RHB model has been introduced in detail in Ref. [22]. The formulism and corresponding computer code for the 3DRHB model with the separable pairing force can be found in Refs. [16, 23, 24]. In the following, we will present the framework very briefly in order to clarify the notations and relevant physical quantities.

The starting point of the point-coupling RHB model is an effective relativistic point-coupling Lagrangian (see e.g., Ref. [25]). For a ground-state even-even nucleus, the RHB equation can be derived as

$$\begin{pmatrix} h_{\rm D}-\lambda & \Delta \\ -\Delta^* & \lambda-h_{\rm D}^* \end{pmatrix}\begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix}=E_\mu\begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix}, \tag{1}$$

where the single-nucleon Dirac Hamiltonian $h_{\rm D}$ reads

$$h_{\rm D}=\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta(M+S)+V, \tag{2}$$

with the scalar S and vector V potentials [25]. The pairing field Δ is determined by the two-body pairing interaction, i.e. the separable pairing force, and the pairing tensor κ. The chemical potential λ is determined by the desired particle number. By solving the RHB Eq. (1) self-consistently, one obtains quasiparticle energies E_μ and the corresponding quasiparticle wave functions $|\mu\rangle$ (the column vectors).

The total binding energy is determined by

$$E_{\rm b}=E_{\rm RHB}+E_{\rm c.m.}+E_{\rm rot}\,, \tag{3}$$

where $E_{\rm RHB}$ is the energy from the RHB part. The microscopic c.m. correction energy $E_{\rm c.m.}$ [17] reads

$$E_{\rm c.m.}=\frac{1}{2MA}\langle\boldsymbol{P}^2_{\rm c.m.}\rangle, \tag{4}$$

with the mass number A and the total momentum $\boldsymbol{P}_{\rm c.m.}$ in the c.m. frame. The rotational correction energy $E_{\rm rot}$ in the cranking approximation [21] reads

$$E_{\rm rot}=\frac{1}{4}\sum_{i=j=1,-1,-2}\frac{\mathcal{M}^{ij}_{(2)}}{\mathcal{M}^{ij}_{(3)}}, \tag{5}$$

$$\mathcal{M}^{ij}_{(n)}=\sum_{\mu,\nu}\frac{|\langle\mu\nu|\hat{Q}_{2i}|\Phi\rangle\langle\mu\nu|\hat{Q}_{2j}|\Phi\rangle|}{(E_\mu+E_\nu)^n}. \tag{6}$$

Here, $|\Phi\rangle$ is the quasiparticle vacuum and the intrinsic quadrupole operators are defined as

$$\hat{Q}_{21}\equiv-2{\rm i}yz;\quad \hat{Q}_{2-1}\equiv-2xz;\quad \hat{Q}_{2-2}\equiv2{\rm i}xy. \tag{7}$$

In the present work, the 3DRHB calculations are performed for even-even Ge isotopes with the point-coupling effective interaction PC-PK1 [25] in the mean-field part and the separable pairing force [15] in the pairing part. The RHB equation (1) is solved by expanding the nucleon spinors U_μ, V_μ in the basis of a three-dimensional harmonic oscillator with 14 major shells in Cartesian coordinates.

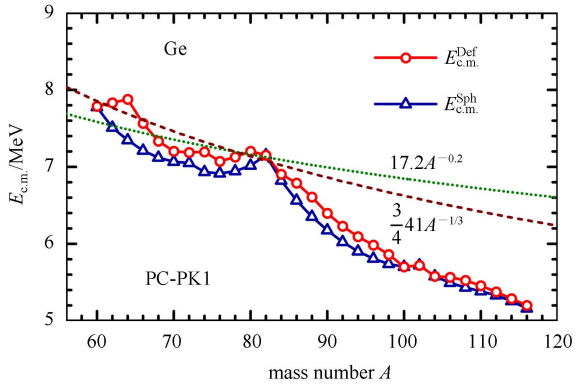

Fig. 1. Microscopic center-of-mass correction energies $E^{\rm Def}_{\rm c.m.}$ of the ground state obtained by the 3DRHB model using the PC-PK1 force [25] (open circles) in comparison with the corresponding results $E^{\rm Sph}_{\rm c.m.}$ of the spherical state (open triangles) as well as two phenomenological formulas [17] (dashed line and dotted line).

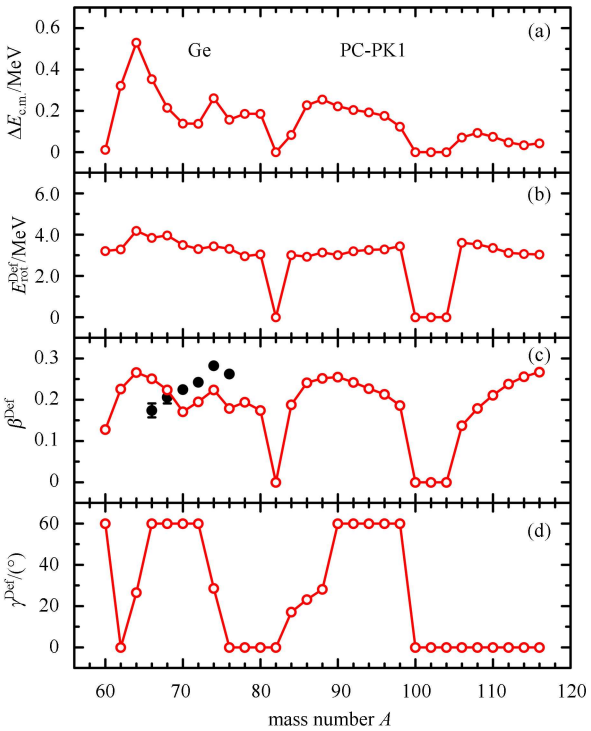

Fig. 2. Difference in the microscopic center-of-mass correction energies $\Delta E_{\rm c.m.}=E^{\rm Def}_{\rm c.m.}-E^{\rm Sph}_{\rm c.m.}$ (a), rotational correction energies $E^{\rm Def}_{\rm rot}$ (b), quadrupole deformations $\beta^{\rm Def}$ (c) and $\gamma^{\rm Def}$ (d) calculated by the 3DRHB model using the PC-PK1 force, in comparison with the available data [27] (solid circles).

3 Results and discussion

Figure 1 displays the calculated microscopic c.m. correction energies $E^{\rm Def}_{\rm c.m.}$ of the ground state in comparison with the corresponding results $E^{\rm Sph}_{\rm c.m.}$ of the spherical state as well as two phenomenological formulas [17]. Detailed numbers for $E^{\rm Def}_{\rm c.m.}$ and $E^{\rm Sph}_{\rm c.m.}$ can be found in the fifth and sixth columns of Table 1, respectively. The microscopic c.m. correction energies vary between 5–8 MeV, and generally decrease as the mass increases. Although the microscopic and the phenomenological methods give similar results for the light nuclei, remarkable differences show up for the nuclei on the neutron-rich side. Moreover, the kick appearing in the microscopic c.m. corrections at $N=50$ ($A=82$), which is related to the shell effect, is also absent in these two phenomenological formulas. One can also see non-negligible differences between $E^{\rm Def}_{\rm c.m.}$ and $E^{\rm Sph}_{\rm c.m.}$, which reflect the deformation effect on the microscopic c.m. correction. This has been specifically discussed for light nuclei in Ref. [26].

In Fig. 2, the calculated difference of the microscopic c.m. correction energies $\Delta E_{\rm c.m.}$, rotational correction energies $E^{\rm Def}_{\rm rot}$, quadrupole deformations $\beta^{\rm Def}$ and $\gamma^{\rm Def}$ are shown in comparison with the available data [27]. The quantitative values are given in Table 1. Obviously, $\Delta E_{\rm c.m.}$ is highly related to the quadrupole deformation parameter $\beta^{\rm Def}$, and generally speaking larger deformation drives more difference between $E^{\rm Def}_{\rm c.m.}$ and $E^{\rm Sph}_{\rm c.m.}$ with only a few exceptions near the neutron-drip line. However, the rotational correction energies $E^{\rm Def}_{\rm rot}$ are rather stable with the typical values 3–4 MeV even though the Ge isotopes present a rapid shape evolution. Of course, there are no rotational corrections for the four spherical nuclei.

Table 1. Total binding energies $E^{\rm Def}_{\rm b}$, rotational correction energies $E^{\rm Def}_{\rm rot}$, microscopic center-of-mass correction energies $E^{\rm Def}_{\rm c.m.}$ and $E^{\rm Sph}_{\rm c.m.}$ (in MeV), quadrupole deformations $\beta^{\rm Def}$ and $\gamma^{\rm Def}$ (in degree) calculated by the 3DRHB model using the PC-PK1 force in comparison with the available data $E^{\rm Exp}_{\rm b}$ [28] and $\beta^{\rm Exp}$ [27]. The superscripts 'Def' and 'Sph' denote the theoretical results of the ground state and the spherical state, respectively.

A	$E^{\rm Exp}_{\rm b}$	$E^{\rm Def}_{\rm b}$	$E^{\rm Def}_{\rm rot}$	$E^{\rm Def}_{\rm c.m.}$	$E^{\rm Sph}_{\rm c.m.}$	$\beta^{\rm Exp}$	$\beta^{\rm Def}$	$\gamma^{\rm Def}$
60		487.34	3.20	7.79	7.78		0.13	60.0
62		517.02	3.28	7.83	7.51		0.23	0.0
64	545.84	545.64	4.18	7.88	7.35		0.27	26.5
66	569.27	568.61	3.85	7.57	7.21	0.17	0.25	60.0
68	590.78	589.84	3.96	7.33	7.12	0.21	0.22	60.0
70	610.51	609.58	3.50	7.20	7.07	0.22	0.17	60.0
72	628.67	628.23	3.30	7.19	7.05	0.24	0.19	60.0
74	645.65	645.95	3.43	7.19	6.93	0.28	0.22	28.6
76	661.59	662.68	3.31	7.07	6.91	0.26	0.18	0.0
78	676.38	678.10	2.96	7.13	6.94		0.19	0.0
80	690.19	691.94	3.04	7.20	7.02		0.17	0.0
82	702.21	700.63	0.00	7.15	7.15		0.00	0.0
84	711.09	711.90	3.01	6.90	6.82		0.19	17.1
86		720.34	2.93	6.79	6.56		0.24	23.2
88		727.86	3.13	6.61	6.35		0.25	28.1
90		734.30	3.01	6.40	6.18		0.25	60.0
92		740.36	3.19	6.23	6.03		0.24	60.0
94		745.67	3.26	6.09	5.90		0.23	60.0
96		750.39	3.29	5.98	5.81		0.21	60.0
98		754.60	3.43	5.86	5.74		0.19	60.0
100		755.12	0.00	5.70	5.70		0.00	0.0
102		759.55	0.00	5.72	5.72		0.00	0.0
104		761.70	0.00	5.58	5.58		0.00	0.0
106		767.42	3.60	5.57	5.49		0.14	0.0
108		769.34	3.53	5.53	5.43		0.18	0.0
110		770.62	3.35	5.46	5.38		0.21	0.0
112		771.34	3.11	5.38	5.33		0.24	0.0
114		771.79	3.06	5.29	5.26		0.26	0.0
116		771.89	3.03	5.20	5.16		0.27	0.0

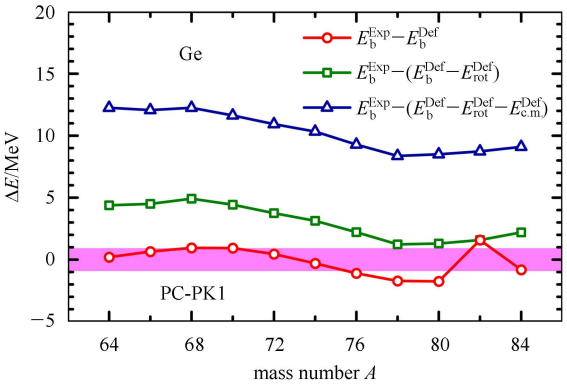

Fig. 3. Discrepancy of the calculated binding energies by the 3DRHB model using the PC-PK1 force with the data [28].

Finally, we discuss the effects of the c.m. correction and rotational correction on the binding energy in Fig. 3, where the discrepancy of the calculated binding energies with the data [28] is shown. Obviously, a large discrepancy (up to ∼10 MeV) is found without both corrections. By taking the c.m. correction into account, the deviations $E_{\rm b}^{\rm Exp}-(E_{\rm b}^{\rm Def}-E_{\rm rot}^{\rm Def})$ (open squares) can be significantly reduced (below ∼5 MeV). After including the rotational correction, the total binding energies $E_{\rm b}^{\rm Def}$ reproduce the data very well and the deviations $E_{\rm b}^{\rm Exp}-E_{\rm b}^{\rm Def}$ (open circles) are mostly between ±1 MeV. Furthermore, we perform a systematic calculation for the binding energies of the even-even isotopes with $20\leqslant Z\leqslant 82$, and find that the root-mean-square deviation with respect to the data is reduced from ∼9 MeV to ∼3 MeV by taking into account the c.m. correction and further down to ∼1 MeV after including the rotational correction.

4 Summary

In summary, we have carried out a systematic investigation of center-of-mass (c.m.) correction and rotational correction in even-even Ge isotopes within the 3DRHB model using the PC-PK1 force. Comparing with the phenomenological formulas, the microscopic c.m. corrections give a kick at $N = 50$, which relates to the shell effect, and remarkable differences show up for the neutron-rich nuclei. A deformation effect on the c.m. correction is also found, which is about several hundred keV. For the rotational correction, the correction energies are rather stable with the typical values 3–4 MeV, even though the Ge isotopes present a rapid shape evolution. By taking the c.m. correction and the rotational correction into account, the calculated binding energies reproduce the data very well and the deviations are mostly between ±1 MeV.

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