DESCRIPTION OF LOW-LYING STRUCTURES IN Gd ISOTOPES WITH COLLECTIVE HAMILTONIAN BASED ON COVARIANT DENSITY FUNCTIONAL THEORY*

Zhi Shi

School of Physics and Nuclear Energy Engineering, Beihang University Beijing 100191, China

Shuangquan Zhang[†]

State Key Laboratory of Nuclear Physics and Technology, School of Physics Peking University, Beijing 100871, China

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The low-lying structures of the even–even Gd isotopes, including the partial dynamical symmetry candidates $^{156-162}$ Gd, are investigated in the framework of five-dimensional collective Hamiltonian based on the covariant density functional theory with the density functional PC-PK1. The available experimental data are reproduced by the microscopic calculations. A shape evolution from the γ -soft 150 Gd to the well-deformed prolate 162 Gd is presented. The ground states of the partial dynamical symmetry candidates $^{156-162}$ Gd are all well-deformed prolate at $\beta \sim 0.35$.

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1. Introduction

The density functional theory (DFT), which starts from an effective nucleon-nucleon interaction and self-consistently determines the nuclear mean-field by all the independent particles inside, has achieved a lot of successes in describing both the nuclear ground state and excited state properties [1–7]. In particular, the covariant version of DFT has the unique advantages that it takes the Lorentz invariance into account from the very

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[†] Corresponding author: sqzhang@pku.edu.cn

beginning, naturally includes the spin-orbit coupling, and provides a consistent description of currents and time-odd fields [1-7]. In recent years, the five-dimensional collective Hamiltonian based on the covariant densityfunctional theory (5DCH-CDFT) [8,9] has been developed and extensively applied to describe the nuclear collective properties, such as the phase transitions [10-14], shape evolutions [15-19] as well as the low-lying spectra along with the isotopic and isotonic chains in different mass regions [8, 20-22].

Dynamical symmetry (DS) plays an important role in the description of complex systems. To describe some specific cases of the breaking of dynamical symmetry, the concepts of partial dynamical symmetry (PDS) [23, 24] and quasi-dynamical symmetry (QDS) [25,26] were introduced. The former takes into account a particular symmetry breaking for which some (but not all) of the virtues of a DS are retained, while the latter is an expression of possibility that can be found in a situation where a subset of physical data may exhibit properties that would result if the system had a symmetry which, in fact, it does not have. Recently, Kremer et al. demonstrated the link between approximate O(6) PDS and SU(3) QDS in the ground state band of ¹⁶⁰Gd, as well as the other eight well-deformed rare-earth isotopes, including ^{156,158}Gd and ¹⁶²Gd [27]. This link has been further demonstrated by Van Isacker [28]. In addition, systematic examinations of SU(3) PDS in finite nuclei have been recently carried out in Refs. [29, 30] and it is found the SU(3) PDS works fairly well for the well-deformed nucleus like ¹⁵⁸Gd but not for the transitional one like 154 Gd [29].

The PDS and QDS has been extensively discussed based on the algebraic Hamiltonian [24–31], therefore it may shed more light on the study of PDS by investigating the PDS candidate nuclei with the microscopic (C)DFT. In the present proceeding, it is reported the description of low-lying structures in Gd isotopes by the 5DCH-CDFT with the covariant density functional PC-PK1 [32].

2. Theoretical framework

A detailed formalism of the 5DCH has been presented in numerous literatures, *e.g.*, see Refs. [33, 34]. The collective Hamiltonian, which simultaneously treats the quadrupole vibrational and rotational excitations, is expressed in terms of the two deformation parameters β and γ , and three Euler angles (ϕ, θ, ψ) $\equiv \Omega$ that define the orientation of the intrinsic principal axes in the laboratory frame

$$\hat{H}_{\text{coll}}(\beta,\gamma) = \hat{T}_{\text{vib}}(\beta,\gamma) + \hat{T}_{\text{rot}}(\beta,\gamma,\Omega) + V_{\text{coll}}(\beta,\gamma).$$
(1)

The three terms in $\hat{H}_{coll}(\beta, \gamma)$ are respective the vibrational kinetic energy

$$\hat{T}_{\text{vib}} = \frac{\hbar^2}{2\sqrt{wr}} \left\{ \frac{1}{\beta^4} \left[\frac{\partial}{\partial\beta} \sqrt{\frac{r}{w}} \beta^4 B_{\gamma\gamma} - \frac{\partial}{\partial\beta} \sqrt{\frac{r}{w}} \beta^3 B_{\beta\gamma} \frac{\partial}{\partial\gamma} \right] + \frac{1}{\beta \sin 3\gamma} \left[-\frac{\partial}{\partial\gamma} \sqrt{\frac{r}{w}} \sin 3\gamma B_{\beta\gamma} \frac{\partial}{\partial\beta} + \frac{1}{\beta} \frac{\partial}{\partial\gamma} \sqrt{\frac{r}{w}} \sin 3\gamma B_{\beta\beta} \frac{\partial}{\partial\gamma} \right] \right\},$$
(2)

the rotational kinetic energy

$$\hat{T}_{\rm rot} = \frac{1}{2} \sum_{k=1}^{3} \frac{\hat{J}_k^2}{\mathcal{I}_k} \,, \tag{3}$$

and the collective potential V_{coll} . \hat{J}_k denote the components of the angular momentum in the body-fixed frame of a nucleus, and the mass parameters $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, as well as the moments of inertia \mathcal{I}_k depend on the quadrupole deformation variables β and γ . Two additional quantities that appear in the \hat{T}_{vib} term (2), $r = B_1 B_2 B_3$ and $w = B_{\beta\beta} B_{\gamma\gamma} - B_{\beta\gamma}^2$, determine the volume element in the collective space.

The eigenvalue problem of the collective Hamiltonian (1) is solved using an expansion of eigenfunctions in terms of a complete set of basis functions that depend on the five collective coordinates β , γ and Ω (ϕ , θ , ψ) [33]. Using the collective wave functions thus obtained

$$\Psi^{IM}_{\alpha}(\beta,\gamma,\Omega) = \sum_{K \in \Delta I} \psi^{I}_{\alpha K}(\beta,\gamma) \Phi^{I}_{MK}(\Omega) , \qquad (4)$$

various observables such as transition probabilities can be calculated.

In the framework of 5DCH-CDFT, the microscopic collective parameters of 5DCH are all determined from the CDFT, which include the mass parameters $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, the moments of inertia \mathcal{I}_k , and the collective potential V_{coll} . The moments of inertia are calculated with the Inglis–Belyaev formula and the mass parameters from the cranking approximation. V_{coll} is obtained by subtracting the zero-point energy corrections from the total energy that corresponds to the solution of constrained triaxial CDFT. A detail formalism can be found in Ref. [8].

3. Results and discussion

First, the constrained calculations on the $\beta - \gamma$ plane with the triaxial covariant density functional theory are preformed for the even-even Gd isotopes from N = 84 to N = 98 with the density functional PC-PK1 [32], and the corresponding potential energy surfaces (PESs) of ^{150,154,158,162}Gd are presented in Fig. 1 to show the shape evolution therein.



Fig. 1. (Color on-line) The potential energy surfaces of 150,154,158,162 Gd in $\beta-\gamma$ plane obtained by constrained triaxial CDFT with PC-PK1. All energies are normalized with respect to the binding energy of the absolute minimum (labeled by white/red dot). The energy difference between the neighboring contour lines is 0.5 MeV.

The ground state of ¹⁵⁰Gd is prolate with $\beta = 0.15$, and its PES around ground state is extremely flat in the γ direction, where a tunnel connecting the prolate and oblate shapes can be seen. With more neutrons, the quadrupole deformation β of Gd isotopes increases to $\beta = 0.3$ for ¹⁵⁴Gd, and to 0.35 for ¹⁵⁸Gd, with the triaxial deformation parameter γ being all kept at $\gamma = 0^{\circ}$. Continuing to add neutrons makes the deformation of the ground state of ¹⁶²Gd very close to that of ¹⁵⁸Gd, *i.e.*, $\beta = 0.35$ and $\gamma = 0^{\circ}$. It is noted that the potential rigidness along both β and γ directions becomes more rigid with the increase of neutron number. Hence, a clear shape evolution from γ -soft to well-deformed prolate can be seen in Gd isotopes, and the ground states of PDS candidates ^{158,162}Gd are found to be with a well-deformed prolate shape. The obtained PESs including the locations of the minima are consistent with the calculations for $^{152-160}$ Gd in Ref. [8] with density functional PC-F1, only that the potentials are slightly more rigid in the γ direction with PC-PK1.

With the collective parameters determined by the CDFT, the excitation energies and the collective wave functions for each value of the total angular momentum I can be obtained by diagonalizing the 5DCH Hamiltonian. Due to the fact that the inertia parameters calculated by the Inglis–Byleav formula systematically underestimate the empirical values, as illustrated in Ref. [8], here the theoretical result of the 2_1^+ state is normalized to the experimental data to obtain the effective moment of inertia used in the collective Hamiltonian.

In Fig. 2, the low-lying excitation energy spectra for the ground state, β and γ bands of ^{150,154,158,162}Gd isotopes calculated by the 5DCH-CDFT are displayed, in comparison with the available data [35]. As shown in Fig. 2, the agreements between the theoretical and experimental energy spectra are overall good. For the ground state bands, with increasing neutron numbers, the theoretical deviations from the experimental data decrease. The ground state bands of ^{158,162}Gd fulfill the relation of I(I + 1), illustrating a SU(3) behavior. For the γ -bands, the 5DCH calculations can also reproduce the data. For the β -bands, although the theoretical results overestimate the energies of bandheads, the increasing trends between the experimental and theoretical results are quite similar.



Fig. 2. (Color on-line) The ground state bands, γ -bands, and β -bands of 150,154,158,162 Gd calculated by the 5DCH-CDFT in comparison with those available data. The theoretical spectra are normalized to the experimental energy of 2^+_1 . The experimental data are taken from the NNDC [35].

More properties on the low-lying spectra of Gd isotopes have been investigated. It is found that the 5DCH-CDFT calculations with PC-PK1 can reproduce the available experimental data for both the $R_{4/2}$ ratios and $B(\text{E2}; 2_1^+ \rightarrow 0_1^+)$ values. By analyzing the 5DCH wave functions, it is found for the ground states of Gd isotopes that the shape fluctuations of β and γ first increase with mass number up to ¹⁵²Gd, then begin to decrease. The average deformation parameters and their shape fluctuations as functions of the angular momentum show a more stable character for the heavier Gd isotopes like ^{158,162}Gd.

To perform an extensive test of a PDS for nuclei in the interacting boson model, a parameter-free quantity, the relative interband B(E2) value ratio from a γ -band state to two states in the ground state band, was examined in Ref. [29]. In Fig. 3, the relative B(E2) ratios calculated by the 5DCH-CDFT are compared with the available data for ^{154,158}Gd isotopes. The data are taken from NNDC [35] and Ref. [29].



Fig. 3. (Color on-line) Comparison of the 5DCH-CDFT predictions with the data on the relative γ -band to ground state band E2 transitions in ^{154,158}Gd. The red/gray (black) bar are the 5DCH-CDFT predictions (data). The largest transition is taken as reference and normalized to 100 for each initial state.

As seen in Fig. 3, the 5DCH-CDFT calculations provide a reasonable description for the relative B(E2) ratios for both ¹⁵⁴Gd and ¹⁵⁸Gd. This agreement is not trivial, as the parameter-free 5DCH-CDFT calculations could not only reproduce the data for the well-deformed nucleus ¹⁵⁸Gd, but also for the transitional nucleus ¹⁵⁴Gd, for which the SU(3) PDS fails to give a reasonable description [29]. For the well-deformed nuclei like ¹⁵⁸Gd, both the microscopic 5DCH-CDFT calculations and the PDS predictions could reproduce the data. As noted in Ref. [29], the main discrepancies for SU(3) PDS to the data are systematic, *i.e.*, PDS systematically underestimate the spin-increasing transitions and overestimate the spin-decreasing transition in the rare-earth region. However, the discrepancies between the data and

the 5DCH-CDFT results are not systematic. This could be explained by the fact that the 5DCH-CDFT calculations have taken the configuration mixing into account self-consistently.

4. Summary

In conclusion, the low-lying structures of the even–even Gd isotopes, including the partial dynamical symmetry candidates ^{156–162}Gd, have been investigated in the framework of 5DCH-CDFT with the density functional PC-PK1. The available experimental data are reproduced by the microscopic calculations. A clear shape evolution from the γ -soft ¹⁵⁰Gd to the well-deformed prolate ¹⁶²Gd has been presented. The shapes of the PDS candidates ^{156–162}Gd are all shown well-deformed prolate with the minima located at $\beta \sim 0.35$. Furthermore, the 5DCH-CDFT calculations not only well describe the relative B(E2) ratios for the PDS candidates, but also work for the transitional nucleus ¹⁵⁴Gd. It is noted that a direct connection between the microscopic theory and the partial dynamical symmetry is unclear. However, it may provide one possible way to explore the hidden dynamical symmetry in the microscopic calculations if one maps the IBM parameters by simulating the potential energy surface obtained from the covariant density functional theory calculations as in Refs. [36, 37].

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