

Skyrme energy-density functional approach to collective modes of excitation in exotic nuclei

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Abstract. Low-frequency collective modes of excitation in neutron-rich nuclei are investigated in the framework of the nuclear energy-density functional method. It is shown that the collective Hamiltonian approach gives the quantitative description of the low-lying states in transitional nuclei with the Skyrme and pairing energy-density functionals as a microscopic input. The inertial functions for large-amplitude vibration and rotation are evaluated by the local normal modes along the axial quadrupole collective coordinate. The time-odd components of the mean fields are fully included in the derived masses.

1. Introduction

Density functional theory has been widely used to describe a variety of quantum many-body systems, including nuclear many-body systems [1]. Ground-state properties including nuclear deformation are described well by the modern nuclear energy-density functional (EDF) method. Experimental evidences of the nuclear shape change are related to the low-lying quadrupole collectivity, such as the ratio of the excitation energy of 2_1^+ and 4_1^+ states, the reduced transition probability $B(E2; 2_1^+ \rightarrow 0_1^+)$, etc.

Magic number or shell closure is an essential concept in understanding the stability against deformation. With the advent of RI beam technology, physics of neutron-rich nuclei has been one of the main current subjects in nuclear physics. It has been revealed that the conventional magic numbers disappear and new magic numbers appear instead in neutron-rich nuclei. Quite recently, the collectivity around $N = 40$ has been extensively studied both experimentally and theoretically. The observed small excitation energy of the 2_1^+ state in neutron-rich Cr isotopes indicates that the deformation develops toward $N = 40$ [2, 3, 4, 5, 6].

In this paper, we demonstrate that the Skyrme-EDF method describes well the low-lying collective states in nuclei undergoing the shape-phase transition.

2. Skyrme-EDF approach for collective excitations using parallel computers

To describe the nuclear deformation and the pairing correlations simultaneously in good account of the continuum, we solve the Hartree-Fock-Bogoliubov (HFB) equations [7] in the coordinate space using cylindrical coordinates. The Skyrme and the density-dependent contact interactions are employed for the particle-hole and particle-particle channels, respectively. We assume axial and reflection symmetries in the ground state. Since the parity (π) and the magnetic quantum number (Ω) are good quantum numbers, the HFB Hamiltonian takes a block diagonal form with



respect to each (Ω^π, q) sector, where q stands for neutron or proton. The HFB equations for each sector are solved independently using parallel computers. Then, the densities and HFB Hamiltonian are updated, which requires the communication among processors. The modified Broyden's method [8] is utilized to calculate new densities. The qp states are truncated according to the qp energy cutoff at $E_\alpha \leq 60$ MeV.

We introduce the additional truncation for the quasiparticle-random-phase approximation (QRPA) calculation in terms of the two-quasiparticle (2qp) energy as $E_\alpha + E_\beta \leq 60$ MeV to reduce the number of 2qp states. The calculation of the QRPA matrix elements in the qp basis is performed in parallel computers. In the present calculation, all the matrix elements are real. For diagonalization of the matrix, we use the ScaLAPACK PDSYEV subroutine. Details of the setup for the HFB+QRPA calculation are given in Ref. [9].

To describe the evolution of the transitional quadrupole collectivity, we need to go beyond the QRPA because the dynamical change of the mean-field potential associated with the large-amplitude collective motion should be taken into account. We thus take the quadrupole collective Hamiltonian approach with the local QRPA (LQRPA) method [10] in the present paper. For evaluation of the collective masses, the LQRPA equations are solved on the constrained HFB states along the collective coordinate. As a collective coordinate, we take the axially symmetric quadrupole deformation β . The collective coordinate is discretized into 20-30 mesh points in the present calculation. The LQRPA equations are solved independently on the discretized points of the collective coordinate. We confirm that the physical quantities calculated by using 20 discretized points get already converged. Details of the model employed and the calculation scheme are given in Ref. [11].

The similar attempts of the EDF-based collective Hamiltonian starting from the Gogny interaction [12, 13], the relativistic Lagrangian [14, 15] and the Skyrme interaction [16] have been made for description of the large-amplitude collective motion. The cranking approximation, however, has been applied to calculate the inertial functions [12, 13, 14, 15, 16], and the time-odd components of the mean field remain largely unexplored except for a few attempts in the adiabatic time-dependent Hartree-Fock-Bogoliubov theories [17, 18, 19]. Our method includes the time-odd mean fields in the inertial functions.

3. Low-lying states in Cr isotopes: Large-amplitude dynamics

We investigated the deformation properties in neutron-rich Cr isotopes with $N = 34 - 44$ employing the constrained HFB method. In ^{58}Cr and ^{60}Cr , the collective potentials are soft against the β deformation even we get the HFB minima at $\beta = 0$. Beyond $N = 38$, the prolate minimum gradually develops up to $N = 44$. We see a shoulder or a shallow minimum at the oblately deformed region as well.

To investigate the effects of the softness of the collective potential on properties of low-lying states in Cr isotopes, the collective Hamiltonian approach with the LQRPA method was employed [11]. When the neutron number increases from ^{58}Cr , the excitation energy of the 2_1^+ state drops toward ^{62}Cr . The ratio of the E_{4+} to E_{2+} ($R_{4/2}$) and the transition probability $B(E2; 2_1^+ \rightarrow 0_1^+)$ grow up at the same time. These features are consistent with the experimental results [4, 5, 6], and it clearly shows the onset of deformation at $N \sim 38$.

We show in Fig. 1(a) the vibrational wave functions squared and in Fig. 1(b) the probability densities that one finds a shape with a specific value of β in the ground state of $^{58-68}\text{Cr}$. The spherical components seen in Fig. 1(a) disappear in Fig. 1(b) due to the moment of inertia $\mathcal{J}(\beta)$ in the volume element.

We discuss the shape evolution of the ground state in detail. In ^{58}Cr , the density is distributed around $\beta = 0$. But it is not sharply localized at the spherical minimum of the potential, which reflects the softness of the collective potential against the deformation. When two neutrons are added to ^{58}Cr , broadening of the density distribution can be seen. When two more neutrons are

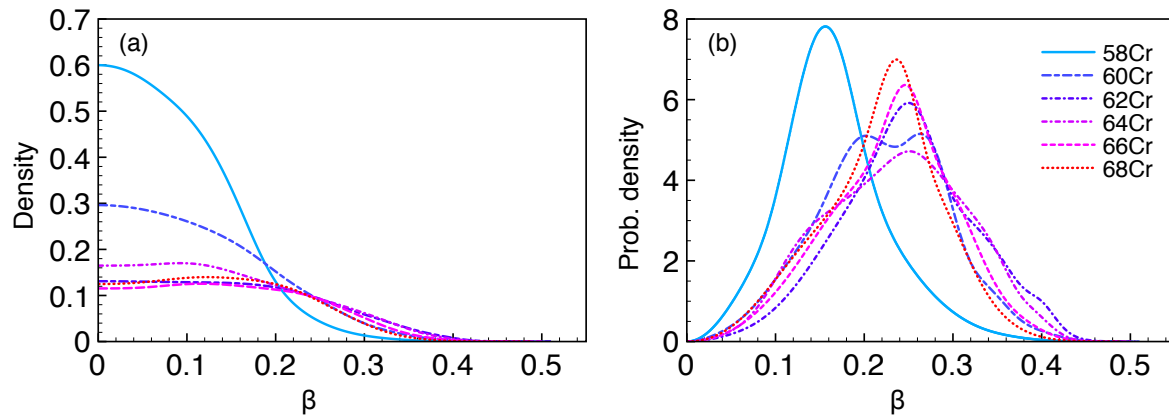


Figure 1. (a) Density and (b) probability-density distributions of the 0_1^+ state in $^{58-68}\text{Cr}$.

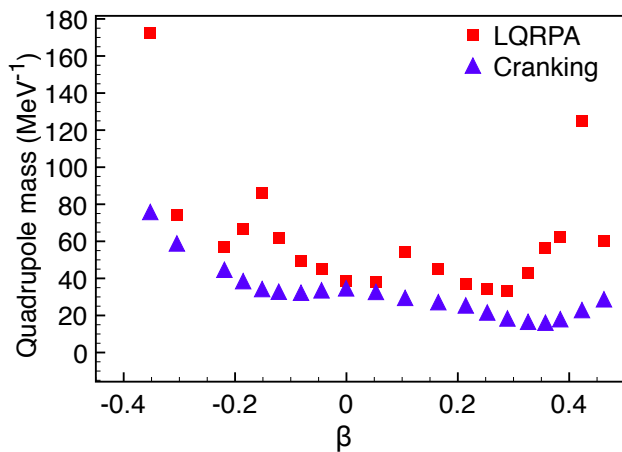


Figure 2. Quadrupole masses as functions of deformation parameter calculated by the LQRPA and the cranking formula in ^{64}Cr .

added, the distribution moves toward a prolately deformed minimum with a large spreading. We see that the distributions in $^{62-68}\text{Cr}$ spread out from the spherical shape to deformed shape with $\beta \simeq 0.4$. We see that the peak in Fig. 1(b) moves toward a larger β in going from ^{58}Cr to ^{62}Cr , and that the peak becomes sharper in $^{66,68}\text{Cr}$. In both figures, we see that the distribution of ^{60}Cr is in between that of ^{58}Cr and of $^{62-68}\text{Cr}$. We can thus say that ^{60}Cr is located close to the critical point of the shape-phase transition in neutron-rich Cr isotopes and the large-amplitude dynamics plays a dominant role.

In our approach, the time-odd components of the mean field are fully included for the calculation of the collective masses. Figure 2 shows the calculated vibrational masses along the collective coordinate. The collective masses calculated by use of the cranking approximation are also shown, where the time-odd components are neglected. The cranking masses show a smooth behavior as functions of the deformation β . In contrast to the cranking masses, the LQRPA masses strongly depend on the deformation, microscopic structure of the collective mode. And the LQRPA masses are larger than the cranking masses.

We see the effects of the time-odd components of the mean field in the excited states. The excited 0_β^+ state in ^{64}Cr is calculated to appear at 1.90 MeV with the LQRPA mass, while we get the 0_β^+ state at 3.38 MeV with the cranking mass. This is due to the larger LQRPA mass than the cranking mass; the collective kinetic energy is much reduced thanks to the time-odd mean field.

4. Summary

We have developed a new framework of the microscopic model for the large-amplitude collective motion based on the nuclear EDF method. The collective masses and the potential appearing in the quadrupole collective Hamiltonian are evaluated by employing the constrained HFB and local QRPA approach, where the time-odd components of the mean field are fully taken into account. We applied this new framework to the shape-phase transition in neutron-rich Cr isotopes around $N = 40$. The present calculation gives consistent results for the low-lying excited states with the observations and the other theoretical approaches. Investigating the collective wave functions, we reach a conclusion that ^{60}Cr is located close to the critical point of the shape-phase transition, and the onset of deformation takes place at $N = 38$. The large-amplitude dynamics plays a dominant role in the shape changes in neutron-rich Cr isotopes.

Systematic calculations with the HFB+QRPA and the collective Hamiltonian approach with the LQRPA method employing the massively paralleled computers for spherical-to-deformed and light-to-heavy nuclei help us not only to understand and to predict new types of collective modes of excitation, but also to shed light on the nuclear EDF of new generations.

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