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Skyrme energy-density functional approach to collective dynamics

Kenichi Yoshida\textsuperscript{1,2}, Nobuo Hinohara\textsuperscript{2}, Takashi Nakatsukasa\textsuperscript{2}

\textsuperscript{1} Department of Physics, Graduate School of Science and Technology, Niigata University, Niigata 950-2181, Japan
\textsuperscript{2} RIKEN Nishina Center for Accelerator-Based Science, Wako, Saitama 351-0198, Japan
E-mail: kyoshida@nt.sc.niigata-u.ac.jp

Abstract. Our recent developments for the microscopic description of nuclear collective dynamics in the framework of the time-dependent density functional theory is presented. It is shown that the quasiparticle random-phase approximation is ready for the systematic investigation of the giant resonances in the entire mass region of nuclear chart and 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. We put emphasis on necessity of the massive use of high performance computers to carry out such microscopic calculations.

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. Furthermore, it is known that nuclear deformation also affects the high-frequency collective modes of excitation, giant resonances (GRs) [2, 3]. For instance, the peak splitting of the giant dipole resonance (GDR), which is caused by the different frequencies of oscillation along the long and short axes, has been observed in experiments [4]. A typical example of the shape phase transition from spherical to deformed ground states and the evolution of deformation splitting in GDRs have been observed in Nd and Sm isotopes [2, 3, 4, 5, 6].

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 $N = 40$ [7, 8, 9, 10, 11].

In this paper, we demonstrate that the Skyrme-EDF method describes well the GDR and 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 \[12\] 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 ($\pi$) and the magnetic quantum number ($\Omega$) are good quantum numbers, the HFB Hamiltonian takes a block diagonal form with respect to each ($\Omega^\pi, q$) 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 \[13\] 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 \texttt{pdsev} subroutine. Details of the setup for the HFB+QRPA calculation are given in Ref. \[14\].

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 \[15\] 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 $\beta$. 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. \[16\].

3. Photoabsorption cross sections of heavy deformed nuclei: Small-amplitude dynamics

Figure 1 shows the photoabsorption cross sections of $^{238}$U. We have a deformation splitting associated with the prolately deformed ground state. We compare it with the experimental data, and we can see that the peak energies are well reproduced. To calculate the QRPA matrix elements and to diagonalize the matrix, it takes about 580 CPU hours and 330 CPU hours, respectively for the $K^\pi = 0^-$ state. Employing 512 processors, we can calculate the total cross sections in 3.5 hours. Our new QRPA calculation code is ready for the systematic investigation of the GRs in all the nuclei.

We apply this new QRPA calculation code to the GDR in Nd and Sm isotopes undergoing the shape-phase transition \[14\]. The Skyrme-HFB calculation reproduces well the evolution of the ground-state deformation; onset of deformation between $N = 84$ and 86, and gradual increase toward $N = 92$. Associated with the ground-state deformation, the isotopic dependence of the peak broadening is well reproduced, surprisingly, even for the transitional nuclei. The width for $N = 82$ and 84 is calculated as $\Gamma = 4.5$ MeV, and it gradually increases to about 6 MeV for $N = 88$, then the splitting becomes visible for $N \geq 90$. Here, the width $\Gamma$ is evaluated by fitting the calculated cross section with a Lorentz line. This broadening effect is commonly interpreted as the mode-mode coupling effects to the low-lying collective modes. In the present QRPA calculation, the mode coupling is not explicitly taken into account. However, the QRPA based on the deformed HFB state may implicitly include a part of the coupling effect.
The GDR peak energies agree well with experimental values. However, a small increase of the width from $^{142}$Nd to $^{144}$Nd observed in the experiment cannot be fully reproduced in the calculation. Since the HFB calculation produces the spherical ground state for $^{144}$Nd, this requires an explicit higher-order calculation beyond the QRPA. We may notice another small disagreement in the peak shape: The calculated GDR peak has a shoulder in the spherical nuclei, and this shoulder is becoming the third peak in the deformed nuclei. This is due to the Landau fragmentation, however, this feature is not clearly observed in the experiments. We found that detailed properties of the Landau fragmentation depend on the choice of the Skyrme EDF. For instance, the fragmentation effect becomes weaker with the SkP functional, to give a better agreement with the experiments.

4. 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 $\beta$ deformation even we get the HFB minima at $\beta = 0$. Beyond $N = 38$, the prolate minimum gradually develops up to $N = 44$. We can 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 is employed [16]. 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 [9, 10, 11], and it clearly shows the onset of deformation at $N \sim 38$.

Evolution of deformation is also seen in the matter radii. In the deformed systems, the increase of radius is proportional to $\beta^2$. Thus, beyond $N = 38$ the radius is constantly larger than the systematics of $A^{1/3}$. Furthermore, we can see that the calculated radius is larger than the HFB result in $^{58}$Cr and $^{60}$Cr associated with the large-amplitude fluctuation. Investigating the collective wave functions, we can discuss more about the dynamics microscopically. In $^{58}$Cr, the wave function is distributed around $\beta = 0$. But the wave function is not sharply localized at the spherical minimum of the potential, which reflects the softness of the collective potential against deformation. When two neutrons are added to $^{58}$Cr, broadening of the wave function can be seen. When two more neutrons are added, the wave function moves toward a prolate relaxed minimum with a large spreading. From this analysis, we can 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.
5. Summary
We have investigated effects of the shape transition on E1 strength distribution in the rare-earth nuclei, using the newly developed parallelized HFB+QRPA calculation code with the Skyrme EDF. This enables us to simultaneously study both high-energy GRs and low-energy collective and non-collective states. The typical characteristics of the GDR for shape-phase transition from spherical to deformed nuclei, especially the isotopic dependence of broadening and splitting of the GDRs, are extremely well reproduced in the calculation.

We have furthermore 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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