Microscopic description of large-amplitude shape-mixing dynamics with local QRPA inertial functions

Nobuo Hinohara*, Koichi Sato†*, Kenichi Yoshida*, Takashi Nakatsukasa* and Masayuki Matsuo**

*Theoretical Nuclear Physics Laboratory, RIKEN Nishina Center, Wako 351-0198, Japan
†Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan
**Department of Physics, Faculty of Science, Niigata University, Niigata 950-2181, Japan

Abstract. We introduce a microscopic approach to derive all the inertial functions in the five-dimensional quadrupole collective Hamiltonian. Local normal modes are evaluated on the constrained mean field in the quasiparticle random-phase approximation in order to derive the inertial functions. The collective Hamiltonians for neutron-rich Mg isotopes are determined with use of this approach, and the shape coexistence/mixing around the $N = 20$ region is analyzed.

Keywords: collective Hamiltonian, large-amplitude collective motion, island of inversion, shape coexistence

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INTRODUCTION

The five-dimensional (5D) quadrupole collective Hamiltonian is a powerful theoretical approach to describe and understand the properties of the low-lying collective states (for a recent review, see Ref. [1]). The collective Hamiltonian consists of, vibrational and rotational kinetic terms, and the model contains six collective inertial functions (three vibrational masses and three rotational moments of inertia), in addition to the collective potential. All the quantities are functions of quadrupole deformation variables $\beta$ and $\gamma$. The collective inertial functions are usually calculated by means of the Inglis-Belyaev (IB) cranking approximation [2], which is derived in the adiabatic perturbation treatment of moving mean field. The most serious shortcoming of the IB approximation is that the time-odd terms of the moving mean field are ignored. To overcome this shortcoming, adiabatic time-dependent Hartree-Fock-Bogoliubov (ATDHFB) theories were developed [3, 4], but the inertial functions derived from ATDHFB theories have not been used in realistic applications so far. Recently we have formulated the constrained Hartree-Fock-Bogoliubov plus local quasiparticle random-phase approximation (CHFB+LQRPA) method [5] to calculate the collective inertial functions on the basis of the adiabatic self-consistent collective coordinate (ASCC) method [6]. This new method enables us to evaluate the inertial functions including the time-odd contribution of the moving field. It has been successfully applied to the oblate-prolate shape coexistence/mixing phenomena in proton-rich Se and Kr isotopes [5, 7].

In this presentation, the large-amplitude deformation dynamics in low-lying states of
neutron-rich Mg isotopes is discussed with the use of the CHFB+LQRPA method. The microscopic mechanism of breaking the \( N = 20 \) shell gap and nature of deformation in this “island of inversion” region is currently under active discussion both experimentally and theoretically. The significant increases of the \( E(4^+)/E(2^+) \) ratio and the \( B(E2; 2^+ \to 0^+) \) value from \(^{30}\text{Mg}\) to \(^{34}\text{Mg}\) clearly indicate a rapid growth of quadrupole deformation. The experimental data suggest a kind of quantum phase transition taking place around \(^{32}\text{Mg}\) and stimulate a microscopic investigation on large-amplitude collective dynamics unique to this region of nuclear chart.

**CHFB+LQRPA METHOD**

The 5D quadrupole collective Hamiltonian is written as

\[
\mathcal{H}_{\text{coll}} = T_{\text{vib}} + T_{\text{rot}} + V(\beta, \gamma),
\]

\[
T_{\text{vib}} = \frac{1}{2} D_{\beta\beta}(\beta, \gamma) \dot{\beta}^2 + D_{\beta\gamma}(\beta, \gamma) \dot{\beta} \dot{\gamma} + \frac{1}{2} D_{\gamma\gamma}(\beta, \gamma) \dot{\gamma}^2 ;
\]

\[
T_{\text{rot}} = \frac{1}{2} \sum_{k=1}^{3} \mathcal{J}_k(\beta, \gamma) \omega_k^2,
\]

where \( V(\beta, \gamma) \) is the collective potential, \( D_{\beta\beta}, D_{\beta\gamma}, \) and \( D_{\gamma\gamma} \) are the vibrational inertial functions, \( \mathcal{J}_k \) are the rotational moments of inertia about three principal axes.

To derive these functions in the 5D quadrupole collective Hamiltonian from the microscopic Hamiltonian \( \hat{H} \), we start from the microscopic theory of large-amplitude collective motion, called the ASCC method [6]. The ASCC method is a theory to extract a collective subspace which is embedded in the large-dimensional time-dependent HFB (TDHFB) manifold. For the present purpose of deriving the 5D collective Hamiltonian, we start from the two-dimensional version of the ASCC method, in which we suppose the existence of a set of two-dimensional canonical collective variables (coordinates and momenta) \((q^1, q^2)\) and \((p_1, p_2)\) describing the vibrational degrees of freedom. The set of two collective coordinates \((q^1, q^2)\) has a one-to-one correspondence to the quadrupole deformation variable set \((\beta, \gamma)\). The CHFB + LQRPA equations are derived from the two-dimensional ASCC method making practical approximations (see Ref. [5] for details of the derivation). The central concept of CHFB + LQRPA method is the local normal modes built on constrained mean field defined at each point of the \((\beta, \gamma)\) plane. The two-dimensional collective space are spanned by CHFB states \(|\phi(\beta, \gamma)\rangle\), which are determined by solving the CHFB equations with four constraints on neutron and proton numbers and quadrupole deformations. The LQRPA equations for vibrational degrees of freedom are written as

\[
\delta \langle \phi(\beta, \gamma) | \hat{H}_{\text{CHFB}}(\beta, \gamma), \hat{Q}^i(\beta, \gamma) \rangle - \frac{1}{i} \hat{P}^i(\beta, \gamma) \langle \phi(\beta, \gamma) | \hat{Q}^i(\beta, \gamma) \rangle = 0,
\]

\[
\delta \langle \phi(\beta, \gamma) | \hat{H}_{\text{CHFB}}(\beta, \gamma), \frac{1}{i} \hat{P}^i(\beta, \gamma) \rangle - \omega_i^2(\beta, \gamma) \langle \phi(\beta, \gamma) | \hat{Q}^i(\beta, \gamma) \rangle = 0.
\]

Here \( \hat{H}_{\text{CHFB}} \) is the microscopic CHFB Hamiltonian including four linear constraint terms, and \( \hat{Q}^i \) and \( \hat{P}^i \) are local infinitesimal generators defined at \((\beta, \gamma)\) with respect
to the CHFB states. There exist a lot of solutions of the LQRPA equations, and we select two LQRPA solutions with the minimal metric criterion; at each point of the \((\beta, \gamma)\) plane, we evaluate the vibrational part of the metric \(W(\beta, \gamma) = D_{\beta \beta}D_{\gamma \gamma} - D_{\beta \gamma}^2\) for all combinations of two LQRPA modes, and find the pair of modes that gives the minimal value. The rotational moments of inertia \(J_k\) are evaluated at each \((\beta, \gamma)\) point using the LQRPA equations for the rotational degrees of freedom:

\[
\delta \langle \phi(\beta, \gamma) | \hat{H}_{\text{CHFB}}(\beta, \gamma), \hat{\Psi}_k(\beta, \gamma) \rangle - \frac{1}{i} \{ \mathcal{J}_k(\beta, \gamma) \}^{-1} \hat{I}_k | \phi(\beta, \gamma) \rangle = 0, \quad (6)
\]

\[
\langle \phi(\beta, \gamma) | [\hat{\Psi}_k(\beta, \gamma), \hat{I}'_k] | \phi(\beta, \gamma) \rangle = i\delta_{kk'} . \quad (7)
\]

**APPLICATION TO THE NEUTRON-RICH Mg ISOTOPES**

**Details of numerical calculation**

Numerical calculations are performed using the pairing-plus-quadrupole (P+Q) Hamiltonian including the quadrupole-pairing interaction. The two-major \(sd\) and \(pf\) shells are taken into account for both neutrons and protons as an active single-particle model space. In order to determine the parameters in the P+Q Hamiltonian, we have performed HFB calculations using the Skyrme SkM* functional and the HFBTHO code [8]. In the Skyrme-HFB calculation, the volume-pairing strength is adjusted to reproduce the experimental neutron pairing gap of \(^{30}\)Ne (1.26MeV). The single-particle energies of the P+Q Hamiltonian are taken from those obtained in the Skyrme-HFB calculation after the effective mass scaling. The strengths of the monopole-pairing interaction are adjusted to reproduce the Skyrme-HFB result at the spherical configuration. The strength of the quadrupole particle-hole interaction are adjusted to reproduce the magnitude of the axial quadrupole deformation at the HFB minimum. The strength of the quadrupole-pairing interaction is determined with the self-consistent prescription [9]. We use the quadrupole polarization charge \(\delta e_{\text{pol}} = 0.5\) for both neutrons and protons when evaluating \(B(E2)\) and quadrupole moments.

**Results**

Figure 1 shows the potential energy surfaces for \(^{30-36}\)Mg determined by solving the CHFB equations. One can clearly see that the prolate deformation grows with increasing neutron number. The potential energy surface for \(^{30}\)Mg is very soft against the axial quadrupole deformation. It has a HFB local minimum at \(\beta = 0.11\). The potential energy surface for \(^{32}\)Mg exhibits a spherical and prolate shape coexistence, where the spherical shape is associated with the neutron shell gap at \(N = 20\). The spherical local minimum disappears in \(^{34-36}\)Mg, and the prolate minima become soft in the triaxial direction.

Figure 2 shows the excitation energies, the spectroscopic quadrupole moments, and the \(E2\) transition strengths, which are obtained by solving the collective Schrödinger
FIGURE 1. Potential energy surfaces of $^{30-36}$Mg.

equation. The calculation well reproduces the experimental trend, such as the lowering of the $2_1^+$ energy and the increase of the $E(4_1^+)/E(2_1^+)$ ratio from $^{30}$Mg to $^{34}$Mg. The behavior of the yrast properties of $^{30-36}$Mg indicates that $^{30}$Mg and $^{32}$Mg are situated in the center of the transitional region of quantum phase transition from spherical to deformed. In particular, it is very interesting to see that the potential energy surface of $^{32}$Mg shows a spherical-prolate shape coexistence. This is a feature somewhat different from the shape phase transition known in the heavy-mass region. The remarkable increase of the $B(E2)$ strength from $^{30}$Mg to $^{36}$Mg agrees with the available experimental data. More detailed analysis including the properties of the excited bands is now in progress.

CONCLUSION

We have developed a practical microscopic method for determining the six inertial functions in the five-dimensional quadrupole collective Hamiltonian. This method is based on the ASCC method and called the CHFB+LQRPA method. This new method has been applied to the large-amplitude shape-mixing dynamics in the yrast bands of neutron-rich Mg isotopes. The result of numerical calculation for excitation energies and $B(E2)$ strengths is in good agreement with the experimental data. It demonstrates that the present method is powerful to describe the large-amplitude quadrupole collective motion in the $^{32}$Mg region as well as the proton-rich Se and Kr isotopes [5, 7]. It also indicates a wide applicability of the CHFB+LQRPA method to various kinds of collec-
FIGURE 2. Excitation energies of the $2^+_1$ and $4^+_1$ states, their ratios, spectroscopic quadrupole moments $Q$ of the $2^+_1$ state, and $B(E2: 2^+_1 \rightarrow 0^+_1)$ values calculated for yrast states in $^{30-36}$Mg. They are compared with the experimental data [10, 11, 12, 13, 14, 15, 16].

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