Microscopic analysis of shape mixing in low-lying states of proton-rich nuclei in the Se-Kr region

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Abstract. Using the five-dimensional quadrupole collective Hamiltonian, we study the oblate-prolate shape coexistence/mixing phenomena in the low-lying states of proton-rich nuclei in the A=70-90 region from a viewpoint of oblate-prolate symmetry and its breaking. To derive the collective Hamiltonian microscopically, we have developed a new method, on the basis of the adiabatic self-consistent collective coordinate method, for determining the collective potential, the vibrational and rotational inertial masses in it. By solving the collective Schrödinger equation, we calculate excitation spectra, spectroscopic quadrupole moments and electric quadrupole transition probabilities among the low-lying states. The result of the calculation clearly indicates the dominant role of the large-amplitude vibration in the triaxial shape degree of freedom. It also exhibits an interesting effect of rotation, which may be called ‘rotational hindrance to the oblate-prolate shape mixing’, that is, the growth of localization of the collective wave function in the (β, γ) deformation space assisted by the rotational motion.

1. Introduction
Shape coexistence phenomena, in which an excited band with a different shape from the ground-band shape exists close in energy to the ground band, are widely observed all over the nuclear chart. In proton-rich Kr isotopes, for example, it has been conjectured that the oblate-prolate shape coexistence occurs since the ground bands which are different from regular rotational spectra [1, 2] and the low-lying excited 0⁺ states [3, 4] were observed. While the observed spectroscopic quadrupole moments [5] suggest the prolate ground state in ⁷⁴,⁷⁶Kr, the ground state of ⁷²Kr is assumed to be oblate from the properties of the E2 transition probabilities [6].

From the mean-field viewpoint, the shape coexistence indicates that there are two equilibrium points in the mean field. In such a case, one may need to take into account the tunneling effects between these local minima. As is well known, the five-dimensional (5D) quadrupole collective Hamiltonian is a powerful tool to treat these large-amplitude collective motions. Recently, we have developed a new method for determining the quadrupole collective Hamiltonian microscopically on the basis of the adiabatic self-consistent collective coordinate (ASCC) method [7, 8].

In this new method, after solving the constrained Hartree-Fock-Bogoliubov (CHFB) equations imposing the constraints on the deformation parameters and the particle numbers, we solve the local QRPA (LQRPA) equations, which is an extension of the usual QRPA (quasiparticle random phase approximation) to non-HFB-equilibrium points, on top of the CHFB states. Therefore, we call this method the CHFB+LQRPA method. One of the advantages of this CHFB+LQRPA...
method is that the inertial masses obtained with this method include the contribution from the time-odd component of the mean field, unlike the widely-used Inglis-Belyaev cranking masses [9, 10]. In this paper, we shall show some results of the application of the CHFB+LQRP A method to shape coexistence in the low-lying states of proton-rich Kr isotopes. More detailed results and discussions are reported in Ref. [11].

2. Theoretical framework

Here, we briefly explain the theoretical framework of the CHFB+LQRP A method (see Ref. [12] for details). The 5D quadrupole collective Hamiltonian is written in terms of the magnitude $\beta$, the degree of triaxiality $\gamma$ of quadrupole deformation, and their time derivatives $\dot{\beta}$ and $\dot{\gamma}$, as

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

where $T_{\text{vib}}$, $T_{\text{rot}}$ and $V$ represent the vibrational, rotational and collective potential energies, respectively. We determine the seven quantities in the collective Hamiltonian, the three vibrational inertial masses, three rotational moments of inertia, and collective potential, by solving the CHFB+LQRP A equations.

In the CHFB+LQRP A method, we first solve the CHFB equation:

$$\delta \langle \phi(\beta, \gamma) \mid \hat{H}_{\text{CHFB}}(\beta, \gamma) \mid \phi(\beta, \gamma) \rangle = 0,$$

to determine the collective potential $V(\beta, \gamma)$. Then, we solve the LQRP A equations on top of the CHFB states obtained above,

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

$$\delta \langle \phi(\beta, \gamma) \mid [\hat{H}_{\text{CHFB}}(\beta, \gamma), \frac{1}{i} \hat{P}_i(\beta, \gamma)] - C_i(\beta, \gamma) \hat{Q}_i(\beta, \gamma) \mid \phi(\beta, \gamma) \rangle = 0, \quad (i = 1, 2).$$

The vibrational inertial functions are calculated by transforming two LQRP A modes to the $(\beta, \gamma)$ degrees of freedom. We also solve the LQRP A equations for rotation to determine the moments of inertia.

3. Numerical results

In this work, we adopt a version of the P+Q interaction which includes the quadrupole pairing interaction as well as the monopole pairing interaction. The interaction parameters are determined as follows: for $^{72}$Kr, we have adjusted the monopole pairing interaction strength $G_0^{(\tau)}$ and the quadrupole particle-hole interaction strength $\chi$ such that the magnitude of the quadrupole deformation $\beta$ and monopole pairing gaps at the oblate and prolate HFB minima obtained in the Skyrme-HFB calculation [13] are approximately reproduced. These values are scaled for $^{74}$Kr and $^{76}$Kr assuming a simple mass number dependence [14]. To determine the quadrupole-pairing strength, we have followed the Sakamoto-Kishimoto prescription [15]. The effective charges are adjusted to $(e_{\text{eff}}^{(n)}, e_{\text{eff}}^{(p)}) = (0.834, 1.834)$ such that the calculated result of $B(E2; 2_1^+ \rightarrow 0_1^+)$ reproduces the experimental value for $^{74}$Kr [5].

Figure 1 shows the collective potentials for $^{72,74,76}$Kr obtained by solving the CHFB equation. All the collective potentials have two local minima: one is prolate and the other is oblate. The
Figure 1. Collective potential energy surfaces $V(\beta, \gamma)$ for $^{72,74,76}$Kr. The regions higher than 5 MeV (measured from the HFB minima) are colored rosy-brown.

Figure 2. LQRPA vibrational inertial mass $D_{\beta\beta}(\beta, \gamma)$ and LQRPA rotational moment of inertia $J_1(\beta, \gamma)$ in unit of MeV$^{-1}$ calculated for $^{72}$Kr. One can see that $D_{\beta\beta}$ indicates strong $\beta - \gamma$ dependence and that the moment of inertia $J_1$ deviates strongly from the irrotational moment of inertia. As we shall see, the $\beta - \gamma$ dependence of the moments of inertia is strongly related to the development of the localization of the collective wave functions. Note that these masses contain the contribution of the time-odd component of the mean field.

spherical shape is a local maximum in all the collective potentials. The experimental data suggest that the ground state is prolate in $^{74,76}$Kr. However, the absolute minimum is oblate in $^{76}$Kr.

We obtain the LQRPA masses for vibration and rotation by solving the LQRPA equation. We depict in Fig. 2 a LQRPA vibrational mass $D_{\beta\beta}$ and rotational moment of inertia $J_1$ for $^{72}$Kr. One can see that $D_{\beta\beta}$ indicates strong $\beta - \gamma$ dependence and that the moment of inertia $J_1$ deviates strongly from the irrotational moment of inertia. As we shall see, the $\beta - \gamma$ dependence of the moments of inertia is strongly related to the development of the localization of the collective wave functions. Note that these masses contain the contribution of the time-odd component of the mean field.

We show the collective wave functions squared $\beta^4|\Phi_{\alpha I}(\beta, \gamma)|^2$ with a factor $\beta^4$ multiplied in Fig. 3. The $\beta^4$ factor carries the dominant $\beta$ dependence of the volume element $G^{1/2}(\beta, \gamma)$. Note that, if the whole volume element was multiplied, all the states would look triaxial because
the factor \( \sin 3\gamma \) in the volume element vanishes on the oblate and prolate lines.

The collective wave function of the ground state has a peak around the oblate potential minimum. However, its tail spreads to the prolate region. The localization of the collective wave function develops as angular momentum increases. In the \( 0^+_1 \) minimum. However, its tail spreads to the prolate region. The localization of the collective function consists of two components: a sharp peak on the oblate side and a component spreading over the prolate region broadly. Although it has a node in the \( \beta \) direction, the \( \gamma \)-vibrational component is strongly mixed. In contrast to the \( 0^+_1 \) state, the collective wave functions of the other yrare states are almost one-dimensional structure and the \( \beta \)-vibrational effects on them are weak. At \( I = 2 \), the vibrational wave function has two peaks both on the oblate and prolate sides. As angular momentum increases, the oblate peak shrinks rapidly and the prolate one grows due to the orthogonality to the yrast states. These behaviors of the collective wave function are consistent with the results of the (1+3)-dimensional ASCC calculation [17, 18], which suggests that the development of the localization of the wave function may be assisted by rotational motion if the moments of inertia have the oblate-prolate asymmetry.

In Fig. 4, the excitation energies and \( B(E2) \) values for \( ^{72}\text{Kr} \) are shown together with the experimental data. We show the result obtained using the IB cranking masses for comparison. The excitation energies obtained with the LQRPA masses are lower than those obtained with the IB masses and in better agreement with the experimental data except for the \( 2^+_1 \) state. In particular, the observed \( 0^+_2 \) excitation energy is close to the \( 2^+_1 \) excitation energy. The excitation energy of the \( 0^+_2 \) state calculated with the LQRPA masses agrees much better with the experimental data.

One can see from the \( E2 \) transition strengths in Fig. 4 that the shape-coexistence-like character becomes stronger with increasing angular momentum: the interband transitions between the initial and final states having equal angular momentum become weaker and weaker, which reflects the growth of the localization of the vibrational wave function in Fig. 3.

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**Figure 3.** Vibrational wave functions squared, \( \beta^4 |\Phi_{\alpha I}(\beta, \gamma)|^2 \), for \( ^{72}\text{Kr} \).
The spectroscopic quadrupole moments for $^{72,74,76}\text{Kr}$ are shown in Fig. 5. In Fig. 5(a), while the signs of the spectroscopic quadrupole moments for $^{72}\text{Kr}$ are positive in the yrast states indicating the oblate-like character, they are negative in the yrare states indicating the prolate-like character. Their magnitude increase with increasing angular momentum, which reflects the development of the localization of the vibrational wave function shown in Fig. 3. The spectroscopic quadrupole moments for $^{74}\text{Kr}$ and $^{76}\text{Kr}$ are shown in Figs. 5(b) and 5(c), respectively. They agree with the experimental data qualitatively well. Their signs and increasing tendency of the magnitude with angular momentum in the ground band are well reproduced. In particular, The spectroscopic quadrupole moments for $^{74}\text{Kr}$ in excellent agreement with the experimental data quantitatively, aside from a minor disagreement for the $2_1^+$ state. However, in $^{76}\text{Kr}$, the absolute values of the quadrupole moments are much smaller than the experimental data. This implies that the magnitude of the quadrupole deformation and/or the localization of the vibrational wave function (not shown here) in the ($\beta, \gamma$) plane are insufficient. The signs of the calculated quadrupole moments in the ground band change from positive in $^{72}\text{Kr}$ to negative in $^{74,76}\text{Kr}$, which indicates a shape transition from the oblate ground state in $^{72}\text{Kr}$ to prolate in $^{74,76}\text{Kr}$.

4. Conclusion
We have studied the oblate-prolate shape coexistence/mixing in the low-lying states of $^{72,74,76}\text{Kr}$ using the 5D quadrupole Hamiltonian determined microscopically by means of the CHFB+LQRPA method, which is based on the 2D ASCC method. Our results indicates a shape transition from the oblate ground state in $^{72}\text{Kr}$ to the prolate ground state in $^{74,76}\text{Kr}$, which is consistent with the experimental data. We have shown that the basic features of the low-lying spectra in these nuclei are determined by the interplay of the large-amplitude shape fluctuation in the $\gamma$ direction, the $\beta$-vibrational excitations, and the rotational motions. Our results suggest that the rotational motion can assist the development of localization of the vibrational wave functions in the ($\beta, \gamma$) deformation space.
Figure 5. Spectroscopic quadrupole moments in unit of $e \text{ fm}^2$ of the first (square), second (circle) and third (triangle) states for each angular momentum in $^{72,74,76}$Kr. Calculated values are shown by open symbols, while experimental data [5] are indicated by filled symbols.

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