MICROSCOPIC DYNAMICS OF SHAPE COEXISTENCE PHENOMENA AROUND ⁶⁸Se AND ⁷²Kr

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Abstract

The adiabatic self-consistent collective coordinate (ASCC) method is applied to the pairing-plus-quadrupole (P + Q) model Hamiltonian including the quadrupole pairing, and the oblate-prolate shape coexistence phenomena in proton-rich nuclei, ⁶⁸Se and ⁷²Kr, are investigated. It is shown that the collective path connecting the oblate and prolate local minima runs along a triaxial valley in the (β , γ) plane. Quantum collective Hamiltonian is constructed and low-lying energy spectra and E2 transition probabilities are calculated for the first time using the ASCC method. Basic properties of the shape coexistence/mixing are well reproduced. We also clarify the effects of the time-odd pair field on the collective mass (inertial function) for the large-amplitude vibration and on the rotational moments of inertia about three principal axes.

1 Introduction

In proton rich nuclei around ⁶⁸Se and ⁷²Kr, oblate–prolate shape coexistence phenomena are observed [1–4]. From the mean-field point of view, the oblate and prolate shapes are mixed by the many-body tunneling through the potential barrier between the two local minima in the potential energy landscape. To describe the shape mixing dynamics, we have to determine the collective degrees of freedom in which direction the large– amplitude shape dynamics takes place. The adiabatic self–consistent collective coordinate (ASCC) method [5] has been proposed as a microscopic theory of large–amplitude collective motion such as the shape coexistence phenomena. This theory is based on the time-dependent Hartree–Fock–Bogoliubov (TDHFB) theory and enables us to extract the collective degrees of freedom in a self–consistent way. In the previous work [6], we have solved the pairing-plus-quadrupole (P + Q) Hamiltonian by means of the ASCC method for ⁶⁸Se and ⁷²Kr nuclei, and successfully extracted the one-dimensional collective path connecting the oblate and prolate local minima. Since the two local minima are mainly connected by the triaxial degrees of freedom, we have suggested that the triaxial deformation plays an essential role in the shape coexistence dynamics of these nuclei.

In this presentation, we report results of the first calculation of low-lying energy spectra and E2 transition probabilities by means of the ASCC method. We derive the quantum collective Hamiltonian that describes the coupled collective motion of the large–amplitude vibration responsible for the oblate–prolate shape mixing and the threedimensional rotation of the triaxial shape. The calculation yields the excited prolate rotational band as well as the oblate ground-state band. It also indicates that the shape mixing decreases as the angular momentum increases.

We also clarify the effect of the time-odd mean-field on the collective mass. This effect is ignored in the cranking mass [7], but is included in the ASCC mass. The time-odd mean-field effect generated by the particle-hole residual interaction was investigated in a few decades ago [8], but those generated by the pairing interaction has not been discussed so far. Quite recently we have shown, using the schematic model Hamiltonian [9], that the time-odd component associated with the quadrupole-type pair field significantly increases the collective mass. In the present calculation, we thus include the quadrupole pairing interaction to the P + Q Hamiltonian to clarify the effect of the time-odd pair field on the collective mass and rotational moments of inertia.

2 The ASCC method

We first recapitulate the basic equations of the ASCC method. The moving-frame TD-HFB state $|\phi(q,p)\rangle = e^{ip\hat{Q}(q)} |\phi(q)\rangle$ is written in terms of the collective coordinate q, and collective momentum p. The TDHFB state is expanded in terms of the collective momentum p under the adiabatic assumption. The collective Hamiltonian is expanded up to the lowest order in p as

$$\mathcal{H}(q, p, \vec{I}) = V(q) + \frac{1}{2}B(q)p^2 + \sum_{i=1}^{3} \frac{I_i^2}{2\mathcal{J}_i(q)},$$
(1)

where the V(q) and B(q) represents the collective potential and the inverse collective mass. We add the rotational energy term with three moments of inertia $\mathcal{J}_i(q)$ to the collective Hamiltonian in order to take into account the rotational motion.

The basic equations of the ASCC method are derived from the adiabatic expansion of the time-dependent variational principle, and are summarized as

$$\delta \langle \phi(q) | H_M(q) | \phi(q) \rangle = 0, \qquad (2)$$

$$\delta \langle \phi(q) | \left[\hat{H}_M(q), \hat{Q}(q) \right] - \frac{1}{i} B(q) \hat{P}(q) | \phi(q) \rangle = 0, \tag{3}$$

$$\delta \langle \phi(q) | [\hat{H}_{M}(q), \frac{1}{i} \hat{P}(q)] - C(q) \hat{Q}(q) - \frac{1}{2B(q)} [[\hat{H}_{M}(q), \frac{dV}{dq}(q) \hat{Q}(q)], \hat{Q}(q)] - \sum_{\tau} \frac{\partial \lambda^{(\tau)}}{\partial q} (q) \hat{N}^{(\tau)} | \phi(q) \rangle = 0.$$
(4)

Equation (2) is called the moving-frame HFB equation, while Eqs. (3) and (4) are called the moving-frame QRPA equations. where $\hat{Q}(q)$ and $\hat{P}(q)$ denote the infinitesimal generators of the collective path,

$$\hat{H}_M(q) = \hat{H} - \sum_{\tau} \lambda^{(\tau)}(q) \hat{N}^{(\tau)} - \frac{dV}{dq}(q) \hat{Q}(q),$$
(5)

is the Hamiltonian in the moving-frame, and $C(q) = \frac{\partial^2 V}{\partial q^2} + \frac{1}{2B(q)} \frac{\partial B}{\partial q} \frac{\partial V}{\partial q}$ is the local stiffness parameter. The operators \hat{H} , $\hat{N}^{(\tau)}$ and the quantity $\lambda^{(\tau)}(q)$ represents the microscopic Hamiltonian, the particle number operators, and the chemical potential, respectively. The QRPA eigenmodes about the HFB equilibrium points, as well as static solutions of the HFB equation, are always special solutions of the ASCC equations. Therefore, the collective path can be constructed by means of the local progression procedure starting from a static HFB state. The collective path at $q + \delta q$ is calculated using the constraint $\langle \phi(q + \delta q) | \hat{Q}(q) | \phi(q + \delta q) \rangle = \delta q$ derived from the canonical variable conditions, if the collective path at q is already known. Repeating this procedure, we can find the collective path and obtain all quantities appearing in the ASCC equations and collective Hamiltonian except the rotational moments of inertia. Three rotational moments of inertia are evaluated by extending the QRPA equations for rotation at the HFB minima to the general HFB states $|\phi(q)\rangle$ on the collective path,

$$\delta \langle \phi(q) | \left[\hat{H}_M(q), i \hat{\Psi}_i(q) \right] - \mathcal{J}_i^{-1}(q) \hat{J}_i | \phi(q) \rangle = 0, \tag{6}$$

where $\hat{\Psi}_i(q)$ and \hat{J}_i are the angle and angular momentum operators in the principal frame.

In the present calculation, we use the P + Q + quadrupole pairing Hamiltonian as a microscopic Hamiltonian \hat{H} . We adopt the same single-particle energies and the P + Q interaction strengths as in Ref. 6 and the self-consistent quadrupole-pairing strength G_2^{self} proposed by Sakamoto and Kishimoto [10].

3 Collective Path

For both ⁶⁸Se and ⁷²Kr, we have found that the lowest HFB state possesses the oblate shape, while second lowest HFB state the prolate shape. We start from the oblate state (q = 0) and determine the collective path connecting the two local minima. Figure 1 shows the collective path projected onto the (β, γ) potential energy surfaces. The path connects the two local minima via the triaxially deformed region. Figure 2 shows various quantities appearing in the collective Hamiltonian and the basic equations of the ASCC method. We define the scale of collective coordinate q by setting $B(q)^{-1} = 1$. The collective mass with respect to the conventional (β, γ) - coordinates is then given by $M(q) = \sqrt{(d\beta/dq)^2 + \beta^2 (d\gamma/dq)^2}^{-1}$. We have found that the collective mass M(q) and three rotational moments of inertia $\mathcal{J}_i(q)$ are enhanced by the time-odd pair field generated by the quadrupole pairing.

4 Energy Spectrum and Transition Probabilities

We requantize the collective Hamiltonian (1) and solve the collective Schrödinger equation

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial q^2} + \frac{1}{2}\sum_{i=1}^3 \mathcal{J}_i^{-1}(q)\hat{I}_i^2 + V(q)\right)\Psi_{IM,k}(q,\Omega) = E_{I,k}\Psi_{IM,k}(q,\Omega),\tag{7}$$

to obtain the excitation energies and collective wavefunctions. The collective wave functions $\Psi_{IM,k}(q,\Omega)$ takes the following form:

$$\Psi_{IM,k}(q,\Omega) = \sum_{K=0}^{I} \Phi_{IK,k}(q) < \Omega | IMK >,$$
(8)

where $\Phi_{IK,k}(q)$ and $\langle \Omega | IMK \rangle$ denote the vibrational wavefunctions and the rotation matrices, respectively. The conventional boundary conditions and symmetry requirements for solving the Bohr collective Hamiltonian [11] are adopted.

Figures 3 display the energy spectrum and B(E2) values for ⁶⁸Se and ⁷²Kr. The calculation yields the excited prolate rotational band as well as the oblate ground-state band. It is seen that the inter-band E2 transitions are weaker than the intra-band E2 transitions, indicating that the oblate-prolate shape coexistence picture holds. The result of calculation also indicates that the oblate-prolate shape mixing decreases as the angular momentum increases. Thus, the basic patterns of oblate-prolate shape coexistence are successfully reproduced in the calculation. The calculation suggest the existence of excited 0^+ state in 68 Se, which is not yet found in experiment. By comparing two calculations, $(G_2 = 0)$ and $(G_2 = G_2^{\text{self}})$, we found that the energy of the 0_2^+ state is much lowered by including the quadrupole pairing interaction. This is due to the enhancement of the collective mass. The energies of the other members of the rotational bands are also lowered, because the quadrupole pairing also enhances the rotational moments of inertia. Experimental data for B(E2) are not available except $B(E2; 2_1^+ \rightarrow 0_1^+) = 1000 \ e^2 \ \text{fm}^4 \ \text{in}^{72} \text{Kr} \ [4].$ Theoretical B(E2) values are calculated using a polarization charge $e_{pol} = 0.881$ that reproduces this data, so that only relative magnitudes should be regarded as theoretical estimates.

In order to estimate the oblate–prolate shape mixing in quantum eigenstates, we define the oblate and prolate probabilities as follows:

$$P_{\rm ob}(I,k) = \int_{q_{\rm min}}^{q_0} dq \sum_{K=0}^{I} |\Phi_{IK,k}(q)|^2, \quad P_{\rm pro}(I,k) = \int_{q_0}^{q_{\rm max}} dq \sum_{K=0}^{I} |\Phi_{IK,k}(q)|^2, \quad (9)$$

where we assume that $q_{\min} \leq q_{ob} < q_0 < q_{pro} \leq q_{max}$. The "boundary" between the oblate and the prolate regions is set to the top of the potential barrier or at $\gamma = 30^{\circ}$. Figure 4 shows these probabilities for ⁶⁸Se and ⁷²Kr. It is clearly seen that the shape mixing rapidly decreases as the angular momentum increases.

5 Summary

For the first time, we have reported the result of calculation of low-lying energy spectra and E2 transition probabilities in ⁶⁸Se and ⁷²Kr by means of the ASCC method. We have derived the quantum collective Hamiltonian that describes the coupled collective motion of the large–amplitude vibration responsible for the oblate–prolate shape mixing and the three-dimensional rotation of the triaxial shape. The calculation yields the excited prolate rotational band as well as the oblate ground–state band. It also indicates that the oblate–prolate shape mixing decreases as the angular momentum increases.

It is surprising that basic pattern of the shape coexistence/mixing phenomena is well reproduced using the one-dimensional collective path running on the two-dimensional (β, γ) plane. Speaking more exactly, this collective path is self-consistently extracted from the huge dimensional TDHB manifold. Namely, the result of calculation indicates that the TDHB collective dynamics of the shape coexistence phenomena in these nuclei is essentially controlled by the single collective variable microscopically derived by means of the ASCC method.

We have also shown that the time-odd pair field enhances the collective mass of the large-amplitude vibrational motion and the rotational moments of inertia. This finding is important in understanding the shape coexistence dynamics, because, together with the collective potential energy, these inertial functions associated with the collective kinetic energies determine the degree of localization of the collective wave function in the (β, γ) plane.

Acknowledgement

This work is supported by the Grant-in-Aid for the 21st Century COE "Center for Diversity and Universality in Physics" from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.

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Figure 1: Collective paths for ⁶⁸Se (*upper*) and ⁷²Kr (*lower*) calculated using the P + Q Hamiltonian including the quadrupole pairing interaction. The paths are projected onto the (β, γ) potential energy surface. The dots in the figures indicate the HB local minima. The equipotential contour lines are drawn every 100 keV.



Figure 2: The monopole pairing gaps, $\Delta_0^{(\tau)}(q)$, the quadrupole pairing gaps, $\Delta_{20}^{(\tau)}(q)$ and $\Delta_{22}^{(\tau)}(q)$, the collective potential V(q), the collective mass M(q), the rotational moments of inertia $\mathcal{J}_i(q)$, the lowest two moving-frame QRPA frequencies squared, $\omega^2(q) = B(q)C(q)$, and the quadrupole deformations, $\beta(q)$ and $\gamma(q)$, are plotted as functions of $\gamma(q)$ for ⁶⁸Se (*upper*) and q for ⁷²Kr (*lower*). Results of two calculations using the P + Q Hamiltonian with ($G_2 = G_2^{\text{self}}$) and without ($G_2 = 0$) the quadrupole pairing interaction are compared.



Figure 3: Excitation energies and B(E2) values for low-lying states of ⁶⁸Se and ⁷²Kr calculated by the ASCC method. In the left (middle) panel, the quadrupole pairing is ignored (included). Experimental data [1–4] are displayed in the right panel. The B(E2) values are given in parentheses beside the arrows in unit of e^2 fm⁴.



Figure 4: The oblate and prolate probabilities evaluated for individual eigenstates in 68 Se (*left*) and 72 Kr (*right*). For each nucleus, the left (right) panel shows values for the lowest (the second lowest) state of each angular momentum. The open (closed) symbols indicate the oblate (prolate) probabilities. The probabilities defined by setting the boundary at the barrier top ($\gamma = 30^{\circ}$) are shown by squares (circles) In each figure, the upper (lower) panel shows the probabilities calculated without (with) including the quadrupole pairing interaction.