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Rotations of Multi-Quasiparticle High-K States

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Abstract. Based on our previous works about the configuration-constrained potential-energy-surface model investigating multi-quasiparticle high-K states, we have further developed the cranking configuration-constrained total Routhian surface method to calculate the collective rotations of the multi-quasiparticle high-K states. The non-axial deformed Woods-Saxon potential has been adopted to obtain single-particle levels. The Woods-Saxon potential gives excellent single-particle level spacing, which is very important for the excitation energy calculations of high-K states. In order to improve pairing calculations, a particle-number-conserving pairing method has been incorporated into the TRS calculation. The calculated moments of inertia can well reproduce experimental values. The structures of the high-K states can be analyzed by the calculations.

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1 Introduction

Atomic nuclei can be excited by breaking nucleon pair(s) [1–3]. If the unpaired nucleons couple to a configuration with a high angular momentum (in fact an angular momentum projection onto the symmetry axis of a deformed nucleus, named K), the excited state can be an isomer due to the forbiddenness of electromagnetic decays from high-K to low-K states [1, 2]. High-K isomers exist in the whole chart of nuclides [1, 2, 4–6]. The specific orbits in multi-quasiparticle states can lead to a shape polarization [7–10]. Therefore, a deformation-variable self-consistent calculation is needed to give quantitative explanations of experimental observations [3, 11].

In our previous works [4–10, 14, 15, 30–36], many high-K states in different mass regions have been investigated by the developed configuration-constrained potential-energy-surface (PES) calculation. However, the PES calculation is limited to multi-quasiparticle states at rest. A high-K state can have collective rotation, leading to a rotational band built on it, called sideband (relative to the

ground-state band). The sidebands of a nucleus provide richer information about nuclear structure than the ground-state band. Theoretically, the calculations of sidebands are difficult due to the non-convergence problem encountered in the cranking Hartree-Fock-Bogoliubov (HFB) model. To overconme the problem, we have developed the particle-number-conserving pairing method which has the merit of the conventional shell model, always giving converged solution for the cranking Hartree-Fock pairing calculation.

2 Model

The calculation starts from the non-axial deformed Woods-Saxon (WS) potential with the universal parameters [12]. The monopole pairing is considered [32]. In order to overcome the non-convergence problem encountered in the cranking Hartree-Fock-Bogoliubov calculation, we have developed the TRS method by using the particle-number-conserving (PNC) pairing method which has the merit of the conventional shell model, always giving converged solution for the cranking Hartree-Fock pairing calculation [26–28].

The total Routhian is written as [29]

$$E^{\omega}(Z,N,\hat{\beta}) = E^{\omega=0}(Z,N,\hat{\beta}) + \Big[\big\langle \hat{H}^{\omega}(Z,N,\hat{\beta})\big\rangle - \big\langle \hat{H}^{\omega=0}(Z,N,\hat{\beta})\big\rangle\Big]. \quad (1)$$

The notations are standard, see [29] for details. The cranked Hamiltonian has the following form [26–28]

$$H_{\rm CSM} = H_{\rm SP} - \omega J_x + H_{\rm P}, \quad (2)$$

where $H_{\rm SP} = \sum_{\xi} h_{\xi}$ with h_{ξ} being the single-particle Hamiltonian with a one-body potential. $-\omega J_x = -\omega \sum j_x$ is the Coriolis force (j_x for the single-particle spin projection onto the x axis perpendicular to the symmetry axis), and $H_{\rm P}$ is the residual two-body pairing interaction,

$$H_{\rm P} = -G \sum_{\xi\eta} a^{\dagger}_{\xi} a^{\dagger}_{\bar{\xi}} a_{\bar{\eta}} a_{\eta}, \quad (3)$$

where ξ ($\bar{\xi}$) and η ($\bar{\eta}$) index the eigen (time-reversed) states of the single-particle Hamiltonian, h_{ξ}. In rotational case, the symmetry of the time reversion is broken, while the signature α, defined by $R_x(\pi) \mid \xi\alpha\rangle = e^{-i\pi\alpha} \mid \xi\alpha\rangle$, keeps being a good quantum number. One can transform the time-reversion representation into the signature basis by [26–28]

$$\beta^{\dagger}_{\xi\alpha=\pm 1/2} = \frac{1}{\sqrt{2}}\{a^{\dagger}_{\xi} \pm \pi a^{\dagger}_{-\xi}\}, \quad (4)$$

where $a^{\dagger}_{-\xi} = (-1)^{\Omega-1/2} a^{\dagger}_{\bar{\xi}}$ with Ω being the single-particle spin projection onto the symmetry axis. The parity "π" keeps conserved. Then we have

$$H_{\rm P} = -G \sum_{\xi\eta} (-1)^{\Omega_{\xi}-\Omega_{\eta}} \beta^{\dagger}_{\xi+} \beta^{\dagger}_{\xi-} \beta_{\eta-} \beta_{\eta+}, \quad (5)$$

where $\xi+$ ($\xi-$) indicates the eigen state ξ with positive (negative) signature [26–28].

The eigen states $|\mu\alpha\rangle$ of the cranked single-particle Hamiltonian, $h_\xi - \omega j_x$,can be expressed as

$$|\mu\alpha\rangle = \sum_\xi c_{\mu\xi}(\alpha)|\xi\alpha\rangle \quad [c_{\mu\xi}(\alpha) \text{ is real}], \tag{6}$$

where $|\xi\alpha\rangle$ stands for the eigen states of the non-cranked single-particle Hamiltonian, h_ξ, while the signature α is conserved. The coefficients $c_{\mu\xi}(\alpha)$ are determined in the diagonalization of the $h_\xi - \omega j_x$ Hamiltonian in the signature basis of the h_ξ Hamiltonian. Correspondingly, a cranked many-particle configuration of the n-body system can be written as a product form

$$|\mu_1\mu_2\cdots\mu_n\rangle = b^\dagger_{\mu_1} b^\dagger_{\mu_2}\cdots b^\dagger_{\mu_n}|0\rangle, \tag{7}$$

where $b^\dagger_{\mu_i}$ is the creation operator for a cranked single-particle state $|\mu_i\alpha\rangle$ (in fact eigen state $|\mu\alpha\rangle$ contains other quantum numbers, e.g., eigen energy $\varepsilon_{\mu\alpha}$ and parity π, but it is sometimes denoted by μ for simplification hereafter). According to Eq. (6), we have

$$b^\dagger_{\mu\pm} = \sum_\xi c_{\mu\xi}(\pm)\beta^\dagger_{\xi\pm}, \tag{8}$$

where the sign "$\pm$" indicates positive or negative signature. In the cranked basis, therefore, the residual two-body paring interaction can be written as [26]

$$H_{\rm P} = -G\sum_{\mu\mu'\nu\nu'} f^*_{\mu\mu'} f_{\nu\nu'} b^\dagger_{\mu+} b^\dagger_{\mu'-} b_{\nu-} b_{\nu'+}, \tag{9}$$

with

$$f^*_{\mu\mu'} = \sum_{\xi\xi'} e^{i\pi\Omega_\xi} c_{\mu\xi}(+) c_{\mu'\xi'}(-), \tag{10}$$

$$f_{\nu\nu'} = \sum_{\eta\eta'} e^{-i\pi\Omega_\eta} c_{\nu\eta}(+) c_{\nu'\eta'}(-). \tag{11}$$

The eigen state of $H_{\rm CSM}$ can be written as [26–28]

$$|\psi^\omega_{\rm CSM}\rangle = \sum_i C_i|i\rangle, \tag{12}$$

with $\{|i\rangle;\, i = 1, 2, \cdots\} = \{|\mu_1\mu_2\cdots\mu_n\rangle;\, \text{scanning}\}$, taking all possible configurations in the truncated cranked many-particle configuration (CMPC) model space, for more details, see Refs. [26–28].

The total cranked shell-model Hamiltonian, $H_{\rm CSM}$, is diagonalized in the CMPC space, i.e., one chooses the eigen states of the no-pairing cranked deformed

Hamiltonian as basis functions for the diagonalization of the total cranked Hamiltonian, $H_{\rm CSM}$ [26]. The cranked deformed basis provides a small but efficient model space for the PNC pairing calculations [27, 28].

The angular momentum of the rotational state $|\psi^{\omega}_{\rm CSM}\rangle$ is calculated by [26]

$$\langle\psi^{\omega}_{\rm CSM}|J_x|\psi^{\omega}_{\rm CSM}\rangle = \sum_i C_i^2\langle i|J_x|i\rangle + 2\sum_{i<j} C_iC_j\langle i|J_x|j\rangle. \qquad (13)$$

The TRS is calculated in a lattice of deformations (β_2, γ, β_4). The γ deformation can appear and play an important role in the descriptions of nuclear collective rotations [13, 16, 17] and high-K excitations [18–22], leading to K mixing [23–25]. The configuration-constrained calculation is achieved by identifying and tracking the given single-particle orbits using calculated average Nilsson numbers. The specific orbits define the multi-quasiparticle high-K configuration.

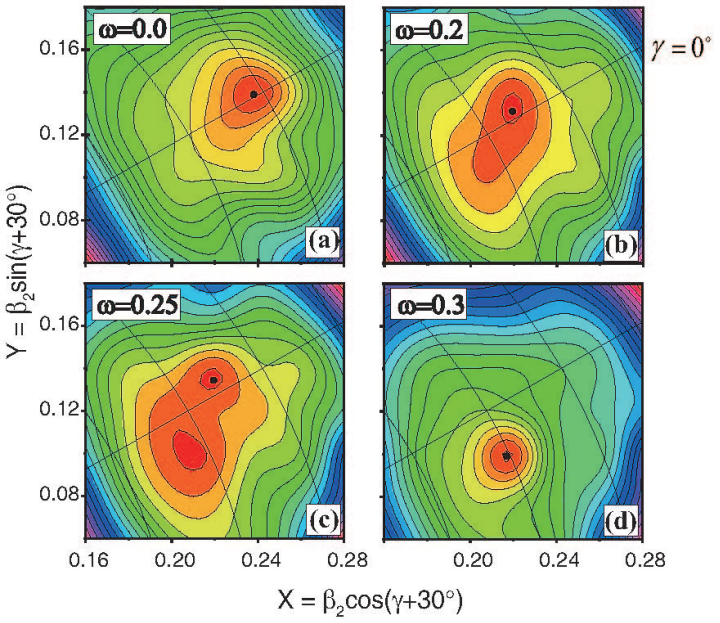

Figure 1. (Color online) Configuration-constrained TRS's for the $K^{\pi} = 15^{+}(\nu\frac{7}{2}^{+}[633] \otimes \nu\frac{7}{2}^{-}[514] \otimes \pi\frac{7}{2}^{+}[404] \otimes \pi\frac{9}{2}^{-}[514])$ band of ^{178}W at different rotational frequencies labeled in each panel. The black dot indicates the minimum which defines the deformation of the multi-qp rotational state. The energy difference between neighboring contours is 100 keV.

3 Calculation

The $A \sim 180$ region is the most known mass region for multi-quasiparticle high-K isomers. As the first calculations of our deformation-pairing-configuration self-consistent TRS model, we have investigated the rotational bands of multi-quasiparticle high-K states in the $A \sim 180$ region. Figure 1 displays the calculated configuration-constrained TRS's for the four-quasiparticle $\nu 7/2^+[633] \otimes 7/2^-[514] \otimes \pi 7/2^+[404] \otimes 9/2^-[514]$ $K^\pi = 15^+$ state, showing deformation evolution with increasing rotational frequency. The high-K state has a prolate deformation at the frequency $\hbar\omega = 0.0$ MeV, and becomes soft with increasing

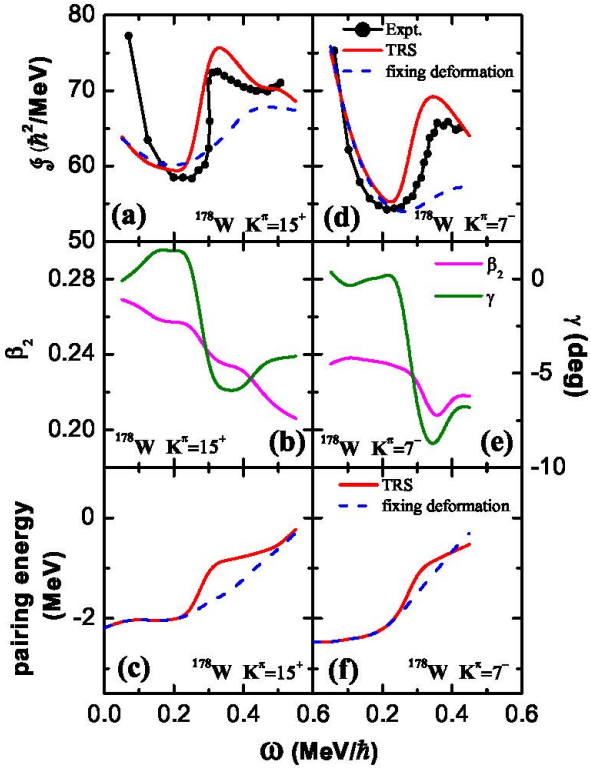

Figure 2. (Color online) Calculated and experimental MoI's[(a),(d)], the corresponding β_2, γ deformations obtained from TRS calculations [(b),(e)], and calculated pairing energies [(c),(f)] for $K^\pi = 15^+(\nu\frac{7}{2}^+[633] \otimes \nu\frac{7}{2}^-[514] \otimes \pi\frac{7}{2}^+[404] \otimes \pi\frac{9}{2}^-[514])$ and $7^-(\nu\frac{7}{2}^+[633] \otimes \nu\frac{7}{2}^-[514])$ bands in ^{178}W. The experimental MoI's are obtained with the data from Refs. [38, 39]. "Fixing deformation" means that the calculation is done with a deformation fixed at that of the bandhead state. The pairing strengths for proton and neutron are $G_p = 0.46$ MeV and $G_n = 0.32$ MeV, respectively. "CSM" is for the usual cranking Woods-Saxon calculation with the LN pairing.

frequency. Two minima appear at $\hbar\omega = 0.25$ MeV, and the state has a $\gamma \approx -6°$ deformation $\hbar\omega \approx 0.3$ MeV.

Figure 2 plots the kinematic moment of inertia (MoI) $\mathcal{J} = J_x/\omega$ and the deformation evolution. It is seen that the MoI calculated by the TRS agrees well with experimental data, reproducing the observed sharp upbending. In order to see the shape-changing effect on rotation, we have made calculations with fixing the shape at $\beta_2 = 0.26, \gamma = 0°$ which is the deformation of the bandhead state of the $K^\pi = 15^+$ band obtained by TRS at $\hbar\omega = 0$. We see that the fixing-deformation calculation gives a quite smooth rotational alignment and significantly smaller MoI compared with experimental data. We see that the deformations (β_2, γ) change with increasing rotational frequency. In order to see the pairing change due to rotational alignment, we extract the pairing energy which is a good measure of the pairing correlation, shown in Figure 2(c). We see that an obvious reduction of the pairing energy occurs in the region of the rotational alignment, which is consistent with the pairing reduction due to alignment, while the fixing-deformation calculation gives a rather smooth reduction of the pairing energy. The cranking HFB calculations collapse around $\hbar\omega \approx 0.35$ MeV [27].

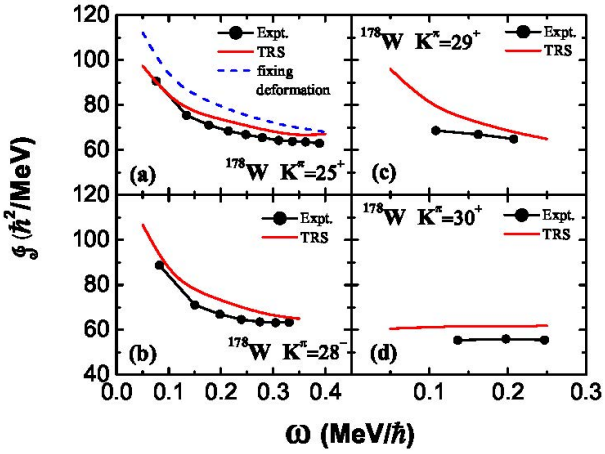

Figure 3. (Color online) Calculated and experimental MoI's for the $K^\pi = 25^+(\nu\frac{5}{2}^-[512] \otimes \nu\frac{7}{2}^-[514] \otimes \nu\frac{7}{2}^+[633] \otimes \nu\frac{9}{2}^+[624] \otimes \pi\frac{1}{2}^-[541] \otimes \frac{5}{2}^+[402] \otimes \pi\frac{7}{2}^+[404] \otimes \pi\frac{9}{2}^-[514])$ (a), $28^-(\nu\frac{1}{2}^-[521] \otimes \nu\frac{7}{2}^-[514] \otimes \nu\frac{7}{2}^+[633] \otimes \nu\frac{9}{2}^+[624] \otimes \pi\frac{1}{2}^-[541] \otimes \frac{11}{2}^-[505] \otimes \pi\frac{7}{2}^+[404] \otimes \pi\frac{9}{2}^-[514])$ (b), $29^+(\nu\frac{5}{2}^-[512] \otimes \nu\frac{1}{2}^-[521] \otimes \nu\frac{7}{2}^-[514] \otimes \nu\frac{7}{2}^+[633] \otimes \nu\frac{9}{2}^+[624] \otimes \nu\frac{7}{2}^-[503] \otimes \pi\frac{1}{2}^-[541] \otimes \frac{5}{2}^+[402] \otimes \pi\frac{7}{2}^+[404] \otimes \pi\frac{9}{2}^-[514])$ (c), and $30^+(\nu\frac{5}{2}^-[512] \otimes \nu\frac{7}{2}^-[514] \otimes \nu\frac{7}{2}^+[633] \otimes \nu\frac{9}{2}^+[624] \otimes \pi\frac{5}{2}^+[402] \otimes \frac{11}{2}^-[505] \otimes \pi\frac{7}{2}^+[404] \otimes \pi\frac{9}{2}^-[514])$ (d) bands in ^{178}W. Experimental data are taken from Refs. [38, 39]. The pairing strengths for proton and neutron are $G_p = 0.46$ MeV and $G_n = 0.32$ MeV, respectively.

^{178}W is a textbook nucleus for the study of high-seniority excitations with many high-K multi-qp states (and their rotational bands) observed up to the highest seniority 10 [37–39]. We have investigated eight-quasiparticle high-K states and their rotations, shown in Figure 3. We see that the deformation-pairing-configuration self-consistent TRS calculations reproduce well the experimental moments of inertia for the collective rotations of various multi-quasiparticle high-K states. The rotational upbendings (alignments) can be explained well.

4 Summary

We have developed the configuration-constrained pairing-deformation-frequency self-consistent TRS calculation in which the paring correlation is treated by the particle-number-conserving method. The typical example for multi-quasiparticle high-K isomers, ^{178}W, has been intensely studied by the model. The experimental moments of inertia have been reproduced well by the present self-consistent TRS calculations. The backbendings or upbendings due to rotational alignments can be understood by the calculations. The detailed evolutions of deformations with increasing frequency and changing configurations are seen from the calculated configuration-constrained TRS. The calculations show that a self-consistent deformation plays an important role in the quantitative description of rotation of a high-K state.

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