Effects of Rotation, Blocking, and Octupole Deformation on Pairing Correlations in U and Pu Isotopes

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Abstract

By introducing octupole correlation interactions into the Nilsson potential and employing the particle-number-conserving method (PNC) within the cranked shell model (CSM) to treat a Hamiltonian containing monopole and quadrupole pairing forces, we investigate the ground-state rotational bands of reflection-asymmetric (RA) nuclei. Based on this, the PNC-CSM calculations reproduce the experimental values of the moments of inertia for the alternating parity bands in even-even nuclei 236,238U and 238,240Pu, as well as for the parity doublet bands in odd-A nuclei 237U and 239Pu in the light actinide region. Compared with the neighboring even-even nuclei 236,238U and 238,240Pu, the moments of inertia of the s = -i intrinsic rotational bands in odd-A nuclei 237U and 239Pu increase by 50% 60%. These increased moments of inertia are mainly caused by the Pauli blocking effect of neutron orbitals near the Fermi surface, which weakens the pairing correlations in the neutron system. In U and Pu isotopes, the slow increase of the moment of inertia with rotational frequency can be interpreted as rotation weakening the pairing correlations of the system. In the low-frequency region, the moment of inertia of reflection-asymmetric nuclei is significantly higher than that of the corresponding reflection-symmetric (RS) nuclei. Moreover, compared with reflection-symmetric nuclei, larger octupole deformation leads to a more pronounced weakening of pairing correlations in reflection-asymmetric nuclear systems.

Full Text

Preamble

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Effects of rotation, blocking and octupole deformation on pairing correlations in the U and Pu isotopes

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Abstract

By incorporating octupole correlations into the Nilsson potential, we investigate the ground-state rotational bands in reflection-asymmetric (RA) nuclei using the cranked shell model (CSM) with monopole and quadrupole pairing correlations treated via a particle-number-conserving (PNC) method. The PNC-CSM calculations successfully reproduce the experimental kinematic moments of inertia (MoIs) for alternating-parity bands in the even-even nuclei ^{236},^{238}U and ^{238},^{240}Pu, as well as parity-doublet bands in the odd-A nuclei ^{237}U and ^{239}Pu. Compared to the neighboring even-even nuclei, the intrinsic s = -i bands in ^{237}U and ^{239}Pu exhibit a 50%-60% increase in $J^{(1)}$, which we attribute primarily to pairing reduction caused by Pauli blocking of the unpaired neutron occupying orbitals near the Fermi surface. The gradual increase of $J^{(1)}$ with rotational frequency can be explained by pairing reduction due to rotation. Our calculations show that the MoIs of reflection-asymmetric nuclei are higher than those of reflection-symmetric (RS) nuclei at low rotational frequencies. Furthermore, compared with RS nuclei, the pairing reduction in RA nuclei becomes more pronounced when larger octupole deformation $_3$ is included in the calculation.

Keywords: octupole correlations; cranked shell model; particle-number-conserving method; alternating-parity bands; parity-doublet bands; pairing correlations

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1 Introduction

Octupole correlations arise from the long-range octupole-octupole interaction between single-particle states with $\Delta l = \Delta j = 3$, leading to intrinsic reflection-asymmetric shapes in ground-state nuclei. The characteristic signatures of octupole correlations in ground-state reflection-asymmetric nuclei include alternating-parity bands in even-mass nuclei and parity-doublet bands in odd-mass nuclei. In the light actinide region, the proton Fermi surface lies between the $f_7/_2$ and $i_{13}/_2$ orbitals, while the neutron Fermi surface lies between the $g_9/_2$ and $j_{15}/_2$ orbitals for nuclei with Z 88 and N 134. The proximity of these levels produces strong octupole coupling.

Experimentally, most odd-mass and even-even nuclei in the actinide region exhibit striking features of octupole correlations. The rotational behaviors of the yrast and negative-parity bands in ^{236,237,238}U and ^{238,239,240}Pu differ significantly, reflecting variations in octupole correlation strength with mass number. Numerous theoretical approaches have been developed to describe octupole correlations in reflection-asymmetric nuclei, including reflection-asymmetric mean-field methods, cluster models, vibrational approaches, the reflection-asymmetric shell model, and the cranked shell model.

In this work, we extend the cranked shell model by treating pairing correlations with a particle-number-conserving method to investigate alternating-parity bands in the even-even nuclei ^{236,238}U and ^{238,240}Pu, along with parity-doublet bands in the odd-A nuclei ^{237}U and ^{239}Pu. In the PNC method, the cranked shell model Hamiltonian is diagonalized directly in a truncated Fock space, thereby exactly conserving particle number and automatically accounting for Pauli blocking effects. Using this PNC-CSM approach, we have conducted a detailed investigation of how rotation, Pauli blocking, and octupole deformation affect pairing correlations in U and Pu isotopes.

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2 Theoretical Framework

Within the cranked shell model framework, the Hamiltonian for an axially deformed nucleus in the rotating frame is given by:

$$H_{\mathrm{CSM}} = H_{\mathrm{Nil}} - \omega J_x + H_{P(0)} + H_{P(2)},$$

where $H_{\mathrm{Nil}} = \sum h_{\mathrm{Nil}}(\varepsilon_2, \varepsilon_3, \varepsilon_4)$ represents the Nilsson Hamiltonian incorporating quadrupole (ε_2), octupole (ε_3), and hexadecapole (ε_4) deformation parameters. The term $-\omega J_x$ describes the Coriolis interaction with rotational frequency ω about the x-axis (perpendicular to the symmetry z-axis).

When $\omega = 0$, the single-particle Hamiltonian h_{Nil} has non-zero matrix elements of Y_{30} between different shells N. Since $p = (-1)^N$, parity is no longer a good quantum number, though Ω (the projection of single-particle angular momentum on the symmetry axis) remains conserved. For $\omega \neq 0$, the system retains symmetry under reflection through the yoz plane, characterized by the S_x operator. Consequently, single-particle orbitals can be labeled by the simplex quantum number s (the eigenvalues of S_x, where $s = \pm i$).

The pairing interaction includes both monopole and quadrupole correlations:

$$H_{P(0)} = -G_0 \sum_{\xi\eta} a_{\xi}^{\dagger} a_{\bar{\xi}}^{\dagger} a_{\bar{\eta}} a_{\eta},$$

$$H_{P(2)} = -G_2 \sum_{\xi\eta} q_2(\xi) q_2(\eta) a_{\xi}^{\dagger} a_{\bar{\xi}}^{\dagger} a_{\bar{\eta}} a_{\eta},$$

where $|\xi\rangle$ ($|\bar{\xi}\rangle$) denotes the time-reversed state of the eigenstate of the Nilsson Hamiltonian h_{Nil}, $q_2(\xi) = \sqrt{16\pi/5}\langle\xi|r^2 Y_{20}|\xi\rangle$ represents the diagonal element of the stretched quadrupole operator, and G_0 and G_2 are the effective strengths of monopole and quadrupole pairing interactions, respectively.

By diagonalizing the cranked shell model Hamiltonian in a sufficiently large cranked many-particle configuration (CMPC) space, we obtain accurate low-lying excited intrinsic states:

$$|\psi\rangle = \sum_i C_i |i\rangle,$$

where $|i\rangle = |\mu_1 \mu_2 \cdots \mu_n\rangle$ is a CMPC for an n-particle system, with $\mu_1 \mu_2 \cdots \mu_n$ representing occupied cranked Nilsson orbitals. Each configuration $|i\rangle$ is characterized by the simplex quantum number $s_i = s_{\mu_1} \cdots s_{\mu_n}$, where s_μ is the simplex of the particle occupying orbital μ. The kinematic moment of inertia for eigenstate $|\psi\rangle$ is:

$$J^{(1)} = \frac{\langle\psi|J_x|\psi\rangle}{\omega}.$$

Experimentally, rotational bands with simplex quantum number s exhibit spin states I of alternating parity according to $p = se^{-i\pi I}$. For reflection-asymmetric systems with even nucleon number, we have $s = +1$ corresponding to $I^\pi = 0^+, 1^-, 2^+, 3^-, \cdots$, and $s = -1$ giving $I^\pi = 0^-, 1^+, 2^-, 3^+, \cdots$. For odd nucleon number systems, $s = +i$ yields $I^\pi = 1/2^+, 3/2^-, 5/2^+, 7/2^-, \cdots$, while $s = -i$ gives $I^\pi = 1/2^-, 3/2^+, 5/2^-, 7/2^+, \cdots$.

The moments of inertia for alternating-parity bands can be expressed as:

$$J_{\pm}^{(1)}(\omega) = \frac{\langle\psi|J_x|\psi\rangle}{\omega} \pm \Delta J^{(1)}(\omega),$$

where $|\psi\rangle$ is the parity-independent wave function at rotational frequency ω obtained from the PNC-CSM method, and $\Delta J^{(1)}(\omega)$ represents the parity splitting of moments of inertia in experimental alternating-parity bands, calculated as:

$$\Delta J^{(1)}(\omega) = \frac{J_{-}^{(1)}(\omega) - J_{+}^{(1)}(\omega)}{2},$$

with $J_-^{(1)}(\omega)$ and $J_+^{(1)}(\omega)$ being the experimental MoIs of negative- and positive-parity rotational bands at frequency ω.

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3 Results and Discussion

3.1 Parameters

In our calculations, the Nilsson parameters (κ, μ) are taken from Ref. [23]. The deformations ε_2, ε_3, and ε_4 serve as input parameters in the PNC-CSM method. The ε_2 and ε_4 values are chosen to match ground-state deformations calculated for the actinide region [24], while the ε_3 values are determined by fitting experimental MoIs and alignments of ground-state bands in U and Pu isotopes.

The deformation parameters $(\varepsilon_2, \varepsilon_3, \varepsilon_4)$ used in our PNC-CSM calculations are: - (0.200, 0.110, -0.055) for ^{236}U - (0.220, 0.130, -0.040) for ^{238}U - (0.228, 0.025, -0.065) for ^{238}Pu - (0.230, 0.010, -0.045) for ^{240}Pu

Deformations for the odd-A nuclei ^{237}U and ^{239}Pu are taken as averages of neighboring even-even nuclei.

The effective pairing strengths G_0 and G_2 can, in principle, be determined from odd-even differences in nuclear binding energies and are connected to the dimensions of the truncated CMPC space. For the even-even nuclei ^{236},^{238}U and ^{238},^{240}Pu, we adopt $G_0^p = 0.25$ MeV, $G_2^p = 0.03$ MeV for protons and $G_0^n = 0.25$ MeV, $G_2^n = 0.015$ MeV for neutrons. For the odd-A nuclei ^{237}U and ^{239}Pu, neutron pairing strengths are slightly smaller than in the even-even cases. For all nuclei studied, the CMPC space is constructed from proton $N = 5, 6$ and neutron $N = 6, 7$ shells, with dimensions of approximately 1000 for both protons and neutrons.

3.2 Moments of Inertia

Figure 1 [Figure 1: see original paper] presents the experimental and calculated kinematic moments of inertia $J^{(1)}$ for alternating-parity bands ($s = +1$) in the even-even nuclei ^{236},^{238}U and ^{238},^{240}Pu, and parity-doublet bands ($s = \pm i$) in the odd-A nuclei ^{237}U and ^{239}Pu. Experimental data for negative- (positive-) parity bands are shown as solid (open) circles. PNC-CSM calculations for reflection-asymmetric nuclei are indicated by black solid lines. After accounting for parity splitting via Eqs. (12) and (13), negative- and positive-parity bands are represented by dash-dotted and dotted lines, respectively. Calculations for reflection-symmetric nuclei (without ε_3 deformation) appear as red dashed lines.

The PNC-CSM calculations reproduce the experimental moments of inertia versus rotational frequency $\hbar\omega$ very well. As shown in Figs. 1(b), 1(c), 1(f), and 1(g), simplex splitting (black solid lines) occurs between $s = +i$ and $s = -i$ partner bands at $\hbar\omega < 0.10$ MeV in both odd-A nuclei ^{237}U and ^{239}Pu. The moments of inertia $J^{(1)}$ increase gradually with rotational frequency in all nuclei. To illustrate this increase more clearly, we examine the differences in MoIs for intrinsic rotational bands in ^{236}U at various rotational frequencies (results for other nuclei are similar). For ^{236}U:

$$\frac{J^{(1)}(^{236}\mathrm{U}, \hbar\omega = 0.30\,\mathrm{MeV}) - J^{(1)}(^{236}\mathrm{U}, \hbar\omega = 0)}{J^{(1)}(^{236}\mathrm{U}, \hbar\omega = 0)} \approx 87.3\%.$$

This demonstrates a substantial increase in $J^{(1)}$ with rising rotational frequency.

To investigate Pauli blocking effects on odd-even differences in MoIs, we compare the MoIs of intrinsic $s = -i$ rotational bands in odd-A nuclei ^{237}U and ^{239}Pu with those in neighboring even-even nuclei ^{236}U and ^{238}Pu at the bandhead ($\hbar\omega = 0.00$ MeV):

$$\frac{J^{(1)}(^{237}\mathrm{U}, \mathrm{RA}) - J^{(1)}(^{236}\mathrm{U}, \mathrm{RA})}{J^{(1)}(^{236}\mathrm{U}, \mathrm{RA})} \approx 61.0\%,$$

$$\frac{J^{(1)}(^{239}\mathrm{Pu}, \mathrm{RA}) - J^{(1)}(^{238}\mathrm{Pu}, \mathrm{RA})}{J^{(1)}(^{238}\mathrm{Pu}, \mathrm{RA})} \approx 49.6\%.$$

Thus, the significant increase in moments of inertia $J^{(1)}$ in odd-A nuclei primarily arises from Pauli blocking effects of the unpaired neutron relative to neighboring even-even nuclei.

Furthermore, as shown in Fig. 1, calculated MoIs for intrinsic rotational bands in reflection-asymmetric nuclei are noticeably higher than those in reflection-symmetric nuclei. To quantify the effect of octupole deformation ε_3 on MoIs, we examine differences between reflection-asymmetric and reflection-symmetric rotational bands at the bandhead ($\hbar\omega = 0.00$ MeV). For U isotopes:

$$\frac{J^{(1)}(^{236}\mathrm{U}, \mathrm{RA}) - J^{(1)}(^{236}\mathrm{U}, \mathrm{RS})}{J^{(1)}(^{236}\mathrm{U}, \mathrm{RS})} \approx 18.7\% \quad (s = +1),$$

$$\frac{J^{(1)}(^{237}\mathrm{U}, \mathrm{RA}) - J^{(1)}(^{237}\mathrm{U}, \mathrm{RS})}{J^{(1)}(^{237}\mathrm{U}, \mathrm{RS})} \approx 24.7\% \quad (s = +i),$$

$$\frac{J^{(1)}(^{237}\mathrm{U}, \mathrm{RA}) - J^{(1)}(^{237}\mathrm{U}, \mathrm{RS})}{J^{(1)}(^{237}\mathrm{U}, \mathrm{RS})} \approx 37.8\% \quad (s = -i),$$

$$\frac{J^{(1)}(^{238}\mathrm{U}, \mathrm{RA}) - J^{(1)}(^{238}\mathrm{U}, \mathrm{RS})}{J^{(1)}(^{238}\mathrm{U}, \mathrm{RS})} \approx 19.7\% \quad (s = +1).$$

For Pu isotopes:

$$\frac{J^{(1)}(^{238}\mathrm{Pu},\mathrm{RA})-J^{(1)}(^{238}\mathrm{Pu},\mathrm{RS})}{J^{(1)}(^{238}\mathrm{Pu},\mathrm{RS})}\approx 17.7\% \quad (s=+1),$$

$$\frac{J^{(1)}(^{239}\mathrm{Pu},\mathrm{RA})-J^{(1)}(^{239}\mathrm{Pu},\mathrm{RS})}{J^{(1)}(^{239}\mathrm{Pu},\mathrm{RS})}\approx 14.3\% \quad (s=+i),$$

$$\frac{J^{(1)}(^{239}\mathrm{Pu},\mathrm{RA})-J^{(1)}(^{239}\mathrm{Pu},\mathrm{RS})}{J^{(1)}(^{239}\mathrm{Pu},\mathrm{RS})}\approx 14.1\% \quad (s=-i),$$

$$\frac{J^{(1)}(^{240}\mathrm{Pu},\mathrm{RA})-J^{(1)}(^{240}\mathrm{Pu},\mathrm{RS})}{J^{(1)}(^{240}\mathrm{Pu},\mathrm{RS})}\approx 20.0\% \quad (s=+1).$$

The differences in U isotopes are generally larger than those in Pu isotopes. In our work, the ε_3 deformations are approximately 0.10 for U isotopes but only about 0.02 for Pu isotopes, clearly demonstrating that ε_3 deformation makes a very important contribution to the increase in moments of inertia $J^{(1)}$.

In general, the increase in $J^{(1)}$ at low frequency and its gradual rise with rotational frequency can be attributed primarily to pairing reduction. To better understand this behavior, we examine in detail how rotation, Pauli blocking, and octupole deformation affect pairing correlations in U and Pu isotopes.

3.3 Pairing Correlations

In the PNC-CSM formalism, the nuclear pairing gap is defined as [25]:

$$\tilde{\Delta}=G_0\sqrt{\langle\psi|H_P|\psi\rangle}.$$

Figure 2 [Figure 2: see original paper] shows the calculated proton and neutron pairing gaps $\tilde{\Delta}$ versus rotational frequency $\hbar\omega$ for alternating-parity bands in even-even nuclei $^{236},^{238}$U and $^{238},^{240}$Pu, and parity-doublet bands in odd-A nuclei ^{237}U and ^{239}Pu. The effective pairing strengths are identical for both reflection-asymmetric and reflection-symmetric calculations. As shown in Fig. 2, pairing gaps in reflection-asymmetric nuclei are generally larger than those in reflection-symmetric nuclei for both protons and neutrons. The pairing gaps decrease with increasing rotational frequency $\hbar\omega$, with particularly significant reductions for neutrons in the odd-A nuclei ^{237}U and ^{239}Pu.

To investigate the effect of rotational frequency on pairing gaps, we examine the relative pairing reduction at $\hbar\omega = 0.30$ MeV compared to the bandhead ($\hbar\omega = 0.00$ MeV) in reflection-asymmetric nuclei. For ^{236}U:

$$\frac{\delta\tilde{\Delta}_p}{\tilde{\Delta}_p(^{236}\mathrm{U},\omega=0)}=\frac{\tilde{\Delta}_p(^{236}\mathrm{U},\hbar\omega=0.30\,\mathrm{MeV})-\tilde{\Delta}_p(^{236}\mathrm{U},\omega=0)}{\tilde{\Delta}_p(^{236}\mathrm{U},\omega=0)}=13.8\%,$$

$$\frac{\delta\tilde{\Delta}_n}{\tilde{\Delta}_n(^{236}\mathrm{U},\omega=0)}=\frac{\tilde{\Delta}_n(^{236}\mathrm{U},\hbar\omega=0.30\,\mathrm{MeV})-\tilde{\Delta}_n(^{236}\mathrm{U},\omega=0)}{\tilde{\Delta}_n(^{236}\mathrm{U},\omega=0)}=12.5\%.$$

Results for other nuclei are similar. For both protons and neutrons, pairing gaps decrease by approximately 10% at $\hbar\omega = 0.30$ MeV compared to the bandhead, leading to the gradual increase of $J^{(1)}$ with rotational frequency in all nuclei.

Comparing Figs. 2(a), 2(d) with Figs. 2(b), 2(e) reveals that neutron pairing gaps decrease significantly in odd-A nuclei ^{237}U and ^{239}Pu. To quantify the Pauli blocking effect on pairing gaps, we examine neutron pairing gaps at the bandhead ($\hbar\omega = 0.00$ MeV):

$$\frac{\delta\tilde{\Delta}_n}{\tilde{\Delta}_n(^{236}\mathrm{U},\mathrm{RA})}=\frac{\tilde{\Delta}_n(^{237}\mathrm{U},\mathrm{RA})-\tilde{\Delta}_n(^{236}\mathrm{U},\mathrm{RA})}{\tilde{\Delta}_n(^{236}\mathrm{U},\mathrm{RA})}=41.0\%,$$

$$\frac{\delta\tilde{\Delta}_n}{\tilde{\Delta}_n(^{238}\mathrm{Pu},\mathrm{RA})}=\frac{\tilde{\Delta}_n(^{239}\mathrm{Pu},\mathrm{RA})-\tilde{\Delta}_n(^{238}\mathrm{Pu},\mathrm{RA})}{\tilde{\Delta}_n(^{238}\mathrm{Pu},\mathrm{RA})}=40.9\%.$$

Neutron pairing gaps decrease by about 40% in odd-A nuclei compared to neighboring even-even nuclei, leading to the significant increase in $J^{(1)}$ observed for the $s = -i$ bands in odd-A nuclei [see Figs. 1(a), 1(c), 1(e), and 1(g)].

To examine the effect of octupole deformation on pairing gaps, we compare pairing gaps at the bandhead ($\hbar\omega = 0.00$ MeV) for ^{236}U and ^{238}Pu with both reflection-asymmetric and reflection-symmetric deformations. For ^{236}U:

$$\frac{\delta\tilde{\Delta}_p}{\tilde{\Delta}_p(^{236}\mathrm{U},\mathrm{RS})}=\frac{\tilde{\Delta}_p(^{236}\mathrm{U},\mathrm{RA})-\tilde{\Delta}_p(^{236}\mathrm{U},\mathrm{RS})}{\tilde{\Delta}_p(^{236}\mathrm{U},\mathrm{RS})}=2.9\%,$$

$$\frac{\delta\tilde{\Delta}_n}{\tilde{\Delta}_n(^{236}\mathrm{U},\mathrm{RS})}=\frac{\tilde{\Delta}_n(^{236}\mathrm{U},\mathrm{RA})-\tilde{\Delta}_n(^{236}\mathrm{U},\mathrm{RS})}{\tilde{\Delta}_n(^{236}\mathrm{U},\mathrm{RS})}=6.6\%.$$

For ^{238}Pu:

$$\frac{\delta\tilde{\Delta}_p}{\tilde{\Delta}_p(^{238}\mathrm{Pu},\mathrm{RS})}=\frac{\tilde{\Delta}_p(^{238}\mathrm{Pu},\mathrm{RA})-\tilde{\Delta}_p(^{238}\mathrm{Pu},\mathrm{RS})}{\tilde{\Delta}_p(^{238}\mathrm{Pu},\mathrm{RS})}=0.6\%,$$

$$\frac{\delta\tilde{\Delta}_n}{\tilde{\Delta}_n(^{238}\mathrm{Pu},\mathrm{RS})}=\frac{\tilde{\Delta}_n(^{238}\mathrm{Pu},\mathrm{RA})-\tilde{\Delta}_n(^{238}\mathrm{Pu},\mathrm{RS})}{\tilde{\Delta}_n(^{238}\mathrm{Pu},\mathrm{RS})}=2.4\%.$$

Pairing gaps decrease in reflection-asymmetric nuclei in PNC-CSM calculations, with larger reductions occurring for greater octupole deformation [see Figs. 2(a) and 2(d)]. Therefore, octupole correlations contribute significantly to the increase in $J^{(1)}$ in reflection-asymmetric nuclei. Results for other nuclei are similar and are not shown.

4 Summary

We have investigated the reflection-asymmetric nuclei ^{236,237,238}U and ^{238,239,240}Pu using the cranked shell model with pairing correlations treated by the particle-number-conserving method. The PNC-CSM calculations successfully reproduce experimental moments of inertia for alternating-parity bands in the even-even nuclei ^{236,238}U and ^{238,240}Pu, and parity-doublet bands in the odd-A nuclei ^{237}U and ^{239}Pu. Our detailed investigation reveals significant effects of rotation, Pauli blocking, and octupole deformation on pairing gaps in these nuclei. The increase in moments of inertia $J^{(1)}$ can be attributed to pairing reduction arising from rotation, Pauli blocking effects, and octupole deformation in the reflection-asymmetric U and Pu isotopes.

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Note: Figure translations are in progress. See original paper for figures.