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Abstract

The recently observed high-spin rotational bands in odd-A nuclei 247,249Cm and 249Cf [Tandel et al., Phys. Rev. C 82 (2010) 041301R] are investigated by using the cranked shell model (CSM) with the pairing correlations treated by a particle-number conserving (PNC) method in which the blocking effects are taken into account exactly. The experimental moments of inertia and alignments and their variations with the rotational frequency are reproduced very well by the PNC-CSM calculations. By examining the -dependence of the occupation probability of each cranked Nilsson orbital near the Fermi surface and the contributions of valence orbitals to the angular momentum alignment in each major shell, the level crossing and upbending mechanism in each nucleus is understood clearly.

Full Text

Preamble

Particle-number conserving analysis of rotational bands in ^{247,249}Cm and ^{249}Cf

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The recently observed high-spin rotational bands in odd-A nuclei ^{247,249}Cm and ^{249}Cf [Tandel *et al.*, Phys. Rev. C 82 (2010) 041301R] are investigated using the cranked shell model (CSM) with pairing correlations treated by a

particle-number conserving (PNC) method in which blocking effects are taken into account exactly. The experimental moments of inertia and alignments and their variations with rotational frequency ω are reproduced very well by the PNC-CSM calculations. By examining the ω-dependence of the occupation probability of each cranked Nilsson orbital near the Fermi surface and the contributions of valence orbitals to angular momentum alignment in each major shell, the level crossing and upbending mechanism in each nucleus is clearly understood.

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Introduction

The rotational spectra of the heaviest nuclei reveal detailed information on single-particle configurations, shell structure, stability against rotation, and thus provide a benchmark for nuclear models. In recent years, in-beam spectroscopy of nuclei with $Z \approx 100$ has been one of the most important frontiers in nuclear structure physics [1]. Besides even-even nuclei [2–4], experimental efforts have also focused on high-spin states of odd-A nuclei, such as ^{253}No [5] and ^{251}Md [6]. Quite recently, rotational bands in odd-A ^{247,249}Cm and ^{249}Cf were observed up to very high spins ($\approx 28\hbar$) and appropriate single-particle configurations have been assigned to these bands [7]. It is worth mentioning that the neutron $\nu 1/2^+[620]$ band in ^{249}Cm is the highest-lying neutron configuration investigated up to such high spins. Although cranking Woods-Saxon calculations reproduced some observed properties well, this experiment, together with previous ones, still challenges nuclear structure models; for example, the absence of alignment of $j_{15/2}$ neutrons in several nuclei in this mass region needs a consistent explanation [7].

In this paper, the cranked shell model (CSM) with pairing correlations treated by a particle-number conserving (PNC) method [8] is used to investigate the rotational bands in ^{247,249}Cm and ^{249}Cf observed in Ref. [7]. Unlike the conventional BCS approach, the PNC method conserves particle number and treats Pauli blocking effects exactly. The PNC-CSM treatment has been used successfully to describe normally deformed and superdeformed high-spin rotational bands in nuclei with $A \approx 160$, 190, and 250 [9–14].

PNC-CSM Formalism

The details of the PNC-CSM treatment can be found in Refs. [9, 10]. For convenience, we briefly summarize the relevant formalism here. The CSM Hamiltonian for an axially symmetric nucleus in the rotating frame is

$$H_{\mathrm{CSM}} = H_0 + H_P = H_{\mathrm{Nil}} - \omega J_x + H_P,$$

where H_{Nil} is the Nilsson Hamiltonian, $-\omega J_x$ is the Coriolis interaction with cranking frequency ω about the x-axis (perpendicular to the nuclear symmetry z-axis), and

$$H_P = H_P^{(0)} + H_P^{(2)}$$

is the pairing interaction. The monopole and quadrupole pairing components are given by

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

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

where $\bar{\xi}$ ($\bar{\eta}$) labels the time-reversed state of a Nilsson state ξ (η), $q_2(\xi) = \sqrt{16\pi/5}\langle\xi|r^2 Y_{20}|\xi\rangle$ is 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.

Instead of the usual single-particle level truncation in conventional shell-model calculations, a cranked many-particle configuration (CMPC) truncation (Fock space truncation) is adopted, which is crucial for making PNC calculations for low-lying excited states both workable and sufficiently accurate [15]. An eigenstate of H_{CSM} can be written as

$$|\Psi\rangle = \sum_i C_i |i\rangle, \quad (C_i \text{ real}),$$

where $|i\rangle$ is a CMPC (an eigenstate of the one-body operator H_0). By diagonalizing H_{CSM} in a sufficiently large CMPC space, accurate solutions for low-lying excited eigenstates are obtained.

The kinematic moment of inertia (MOI) for the state $|\Psi\rangle$ is

$$J^{(1)} = \frac{\langle\Psi|J_x|\Psi\rangle}{\omega} = \frac{1}{\omega}\left(\sum_i C_i^2 \langle i|J_x|i\rangle + 2\sum_{i<j} C_i C_j \langle i|J_x|j\rangle\right).$$

Considering J_x to be a one-body operator, the matrix element $\langle i|J_x|j\rangle$ for $i \neq j$ is nonzero only when $|i\rangle$ and $|j\rangle$ differ by one particle occupation [9, 10]. After a certain permutation of creation operators, $|i\rangle$ and $|j\rangle$ can be recast into $|i\rangle = (-1)^{M_{i\mu}}|\mu\cdots\rangle$ and $|j\rangle = (-1)^{M_{j\nu}}|\nu\cdots\rangle$, where the ellipsis stands for the same particle occupation and $(-1)^{M_{i\mu(\nu)}} = \pm 1$ according to whether the permutation is even or odd. Therefore, the angular momentum alignment of $|\Psi\rangle$ can be expressed as

$$\langle\Psi|J_x|\Psi\rangle = \sum_{\mu} j_x(\mu) + \sum_{\mu<\nu} j_x(\mu\nu).$$

The diagonal contribution is $j_x(\mu) = \langle\mu|j_x|\mu\rangle n_\mu$, where $n_\mu = \sum_i |C_i|^2 P_{i\mu}$ is the occupation probability of the cranked Nilsson orbital $|\mu\rangle$ and $P_{i\mu} = 1$ (0) if $|\mu\rangle$ is occupied (empty). The off-diagonal (interference) contribution is $j_x(\mu\nu) = 2\langle\mu|j_x|\nu\rangle \sum_{i<j}(-1)^{M_{i\mu}+M_{j\nu}} C_i C_j$.

Parameters and Calculational Details

The Nilsson parameter systematics (κ, μ) [16, 17] cannot reproduce well the order of single-particle levels for very heavy nuclei with $A \approx 250$ (see, e.g., Ref. [14]). Recently we have proposed a new set of (κ, μ) parameters given in Table I, obtained by fitting the observed single-particle spectra of all known odd-A nuclei in this mass region [18]. Note that readjustment of Nilsson parameters is also necessary in other regions of the nuclear chart [19, 20].

The deformation parameters $(\varepsilon_2, \varepsilon_4)$ are $(0.242, 0.002)$ for ^{247}Cm and $(0.248, 0.008)$ for ^{249}Cm and ^{249}Cf. There are no experimental values for these parameters. The values used in various calculations or predicted by different models differ. Those adopted here are larger than those used in Ref. [7] or predicted in Ref. [21], and smaller than the interpolated values from Ref. [22] where, for example, the ϵ_2 values for ^{248}Cf and ^{250}Cf are 0.260 and 0.265, respectively.

The effective pairing strengths can, in principle, be determined by odd-even differences in binding energies and are connected with the dimension of the truncated CMPC space. The CMPC space for these very heavy nuclei is constructed in the proton $N = 4, 5, 6$ shells and neutron $N = 6, 7$ shells. The dimensions of the CMPC space are about 1000 for both protons and neutrons in our calculations. The corresponding effective monopole and quadrupole pairing strengths are $G_{0p} = 0.50$ MeV and $G_{2p} = 0.04$ MeV for protons, and $G_{0n} = 0.30$ MeV and $G_{2n} = 0.02$ MeV for neutrons. The stability of PNC calculation results against changes in CMPC space dimension has been investigated in Refs. [9, 11, 15]. In the present calculations, almost all CMPCs with weight $> 0.1\%$ are taken into account, so the solutions for low-lying excited states are accurate enough. A larger CMPC space with renormalized pairing strengths gives essentially the same results.

Results and Discussion

Figure 1 [Figure 1: see original paper] shows the calculated cranked Nilsson levels near the Fermi surface of ^{247}Cm. Positive (negative) parity levels are denoted by blue (red) lines. Signature $\alpha = +1/2$ ($\alpha = -1/2$) levels are denoted by solid (dotted) lines. For both protons and neutrons, the sequence of single-particle levels near the Fermi surface matches experimental data from ^{247}Cm and ^{247}Bk [1], with the only exception being the $\nu 5/2^+[622]$ orbital. Many theoretical models predict that the first excited state in $N = 151$ isotones should be $\nu 7/2^+[624]$ (see, e.g., Ref. [23]), which is inconsistent with experimental results showing $\nu 5/2^+[622]$ as the first excited state. The low excitation energy of the $\nu 5/2^+[622]$ state in $N = 151$ isotones has been interpreted as a consequence of a low-lying $K^\pi = 2^-$ octupole phonon state [24]. Figure 1 shows a proton gap at $Z = 96$ and a neutron gap at $N = 152$, consistent with experiment and Woods-Saxon potential calculations [25]. The cranked Nilsson levels of ^{249}Cm and ^{249}Cf are quite similar to those of ^{247}Cm and are not shown here.

Figure 2 [Figure 2: see original paper] shows the experimental and calculated MOIs and alignments for the ground state bands (gsb' s) in ^{247,249}Cm and ^{249}Cf. Experimental MOIs and alignments are denoted by solid squares (signature $\alpha = +1/2$) and open squares (signature $\alpha = -1/2$), while calculated values are denoted by solid lines (signature $\alpha = +1/2$) and dotted lines (signature $\alpha = -1/2$). The experimental MOIs and alignments of all three 1-quasiparticle bands are well reproduced by the PNC-CSM calculations, which strongly supports the configuration assignments for these high-spin rotational bands adopted in Ref. [7]. Moreover, the signature splitting in the $\nu 1/2^+[620]$ band is also well reproduced, which is understandable from the behavior of the cranked Nilsson orbital $\nu 1/2^+[620]$ in Fig. 1. The upbending frequency $\hbar\omega_c \sim 0.25$ MeV for the gsb in ^{249}Cf is slightly larger than that of the Cm isotopes ($\hbar\omega_c \sim 0.20$ MeV). These results agree well with experiment and cranking Woods-Saxon calculations [7].

One advantage of the PNC method is that the total particle number $N = \sum_\mu n_\mu$ is exactly conserved, while the occupation probability n_μ for each orbital varies with rotational frequency $\hbar\omega$. By examining the ω-dependence of orbitals close to the Fermi surface, one can learn how Nilsson levels evolve with rotation and gain insight into the upbending mechanism. Figure 3 [Figure 3: see original paper] shows the occupation probability n_μ of each orbital μ near the Fermi surface for the gsb' s in ^{249}Cm and ^{249}Cf. The top and bottom rows show protons and neutrons, respectively. Positive (negative) parity levels are denoted by blue solid (red dotted) lines.

From Fig. 3(a), the occupation probability of $\pi 7/2^+[633]$ ($i_{13/2}$) drops gradually from 0.5 to nearly zero as the cranking frequency increases from about 0.20 MeV to 0.30 MeV, while occupation probabilities of some other orbitals slightly increase. This can be understood from the cranked Nilsson levels shown in Fig. 1(a). The $\pi 7/2^+[633]$ orbital is slightly above the Fermi surface at $\hbar\omega = 0$. Due to pairing correlations, this orbital is partly occupied. With increasing $\hbar\omega$, this orbital moves farther above the Fermi surface, so after the band-crossing frequency its occupation probability becomes smaller. Meanwhile, occupation probabilities of orbitals approaching the Fermi surface increase with $\hbar\omega$. This phenomenon is even clearer in Fig. 3(b), but the band-crossing occurs at $\hbar\omega_c \sim 0.25$ MeV, slightly larger than in ^{249}Cm. Thus, band-crossings in both cases are mainly caused by the $\pi i_{13/2}$ orbitals.

In Fig. 3(c), with increasing $\hbar\omega$ the occupation probability of $\nu 1/2^+[620]$ decreases slowly while that of the high-Ω (deformation-aligned) $\nu 9/2^-[734]$ orbital ($j_{15/2}$) increases slowly, indicating only a small neutron contribution to upbending for the gsb in ^{249}Cm. In Fig. 3(d), the neutron orbital $\nu 9/2^-[734]$ of $j_{15/2}$ parentage is completely blocked by an odd neutron, so it contributes nothing to upbending for the gsb in ^{249}Cf.

The contribution of each proton and neutron major shell to the angular momentum alignment $\langle J_x \rangle$ for the gsb' s in ^{249}Cm and ^{249}Cf is shown in Fig. 4 [Figure 4: see original paper]. The diagonal $\sum_\mu j_x(\mu)$ and off-diagonal parts $\sum_{\mu<\nu} j_x(\mu\nu)$ from the proton $N = 6$ and neutron $N = 7$ shells are shown by dotted lines. Note that in this figure, the smoothly increasing part of the alignment represented by the Harris formula ($\omega J_0 + \omega^3 J_1$) is not subtracted (cf. Fig. 2 caption). It is clear that upbendings for the gsb' s in ^{249}Cm at $\hbar\omega_c \sim 0.20$ MeV and in ^{249}Cf at $\hbar\omega_c \sim 0.25$ MeV mainly come from the proton $N = 6$ shell. Furthermore, the upbending for the gsb in ^{249}Cm arises primarily from the off-diagonal part of the proton $N = 6$ shell, while both diagonal and off-diagonal parts of the proton $N = 6$ shell contribute to upbending for the gsb in ^{249}Cf.

For a clearer understanding of the upbending mechanism, Fig. 5 [Figure 5: see original paper] presents contributions of intruder proton orbitals $i_{13/2}$ (top row) and intruder neutron orbitals $j_{15/2}$ (bottom row) to the angular momentum alignments $\langle J_x \rangle$. The diagonal (off-diagonal) part $j_x(\mu)$ [$j_x(\mu\nu)$] is denoted by blue solid (red dotted) lines. Near the proton Fermi surfaces of Cm and Cf isotopes, the proton $i_{13/2}$ orbitals are $\pi 3/2^+[651]$, $\pi 5/2^+[642]$, and $\pi 7/2^+[633]$. Other orbitals of $\pi i_{13/2}$ parentage are either fully occupied or fully empty (cf. Fig. 3) and contribute nothing to upbending.

In Fig. 5(a), the PNC calculation shows that after upbending ($\hbar\omega \geq 0.20$ MeV) the off-diagonal part $j_x(\pi 5/2^+[642] \otimes \pi 7/2^+[633])$ changes significantly. The alignment gain after upbending mainly comes from this interference term. The off-diagonal part $j_x(\pi 3/2^+[651] \otimes \pi 5/2^+[642])$ and the diagonal part $j_x(\pi 7/2^+[633])$ also contribute slightly to upbending in ^{249}Cm. From Fig. 5(b), for ^{249}Cf the main contribution to alignment gain after upbending comes from the diagonal part $j_x(\pi 7/2^+[633])$ and the off-diagonal part $j_x(\pi 5/2^+[642] \otimes \pi 7/2^+[633])$. Again, this confirms that upbending in both cases is mainly caused by the $\pi i_{13/2}$ orbitals.

The absence of $j_{15/2}$ neutron alignment in nuclei of this mass region can be understood from the contribution of intruder neutron orbitals ($N = 7$) to $\langle J_x \rangle$. For nuclei with $N \approx 150$, among neutron orbitals of $j_{15/2}$ parentage, only the high-Ω (deformation-aligned) $\nu 7/2^-[743]$ and $\nu 9/2^-[734]$ are close to the Fermi surface. The diagonal parts of these two orbitals contribute no alignment to upbending; only interference terms contribute slightly if the neutron $j_{15/2}$ orbital is not blocked [cf. Fig. 5(c)].

Summary

In summary, the recently observed high-spin rotational bands in odd-A nuclei ^{247,249}Cm and ^{249}Cf [7] have been investigated using the PNC-CSM. In the PNC treatment of pairing correlations, particle number is conserved and blocking effects are taken into account exactly. The experimental ω-variations of MOIs and alignments are reproduced very well by the PNC-CSM calculations. By analyzing the ω-dependence of occupation probabilities of cranked Nilsson orbitals near the Fermi surface and the contributions of valence orbitals in each major shell to angular momentum alignment, the level crossing and upbending mechanisms in each nucleus are clearly understood. Upbending in the ground state rotational bands of these nuclei is mainly caused by intruder proton ($N = 6$) $\pi i_{13/2}$ orbitals. The reason for the absence of $j_{15/2}$ neutron alignment is discussed.

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