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Abstract

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Full Text

Preamble

Systematic Investigation of Rotational Bands in Nuclei with $Z = 100$ Using a Particle-Number Conserving Method Based on a Cranked Shell Model

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The rotational bands in nuclei with $Z \leq 100$ are investigated systematically using a cranked shell model (CSM) with pairing correlations treated by a particle-number conserving (PNC) method, in which blocking effects are taken into account exactly. By fitting the experimental single-particle spectra in these nuclei, a new set of Nilsson parameters (ϵ and μ) and deformation parameters (β and γ) are proposed. The experimental kinematic moments of inertia for rotational bands in even-even, odd-A, and odd-odd nuclei, and the bandhead energies of the one-quasiparticle bands in odd-A nuclei, are reproduced quite well by the PNC-CSM calculations. By analyzing the β -dependence of the occupation probability of each cranked Nilsson orbital near the Fermi surface and the contributions of valence orbitals in each major shell to the angular momentum alignment, the upbending mechanism in this region is clearly understood.

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Introduction

Since the importance of shell effects on the stability of superheavy nuclei (SHN) was illustrated [1] and the existence of an island of stability of SHN was predicted around $Z = 114$ and $N = 184$ [2-5], considerable efforts have focused on the exploration of SHN. Great experimental progress has been made in synthesizing superheavy elements (SHE). Up to now, SHEs with $Z \leq 118$ have been synthesized via cold and hot fusion reactions [6-8]. However, these SHN are all neutron-deficient with neutron numbers at least 7 less than the predicted next neutron magic number 184. Therefore, one still cannot make a definite conclusion about the location of the island of stability.

The single-particle shell structure is crucial for determining the location of the island of stability. For example, whether the next shell closure for protons appears at $Z = 114$ or 120 is mainly determined by the splitting of the spin doublets $2f_{7/2}$ and $2f_{5/2}$. Experimentally, one cannot directly investigate the single-particle level structure of SHN with $Z \leq 110$ because the production cross sections of these nuclei are tiny, making spectroscopy experiments impossible at present. Theoretically, different models usually predict different closed shells beyond ^{208}Pb ; even within the same model there are parameter-dependent predictions [9]. For example, macroscopic-microscopic models or the extended Thomas-Fermi-Strutinsky integral approach predict that the next shell closure for protons is at $Z = 114$ [10-12]; relativistic mean-field models predict $Z = 114$ or 120 as the next proton magic number [13-16]; predictions from nonrelativistic mean-field models with Skyrme forces range from $Z = 114, 120, 124$, to 126, depending on

the parametrization [13]. The shell structure of SHN is important not only for locating the island of stability but also for studying the synthesis mechanism of SHN [17-26], particularly the survival probability of excited compound nuclei [27, 28].

To learn more about the shell structure of SHN, an indirect approach is to study lighter nuclei in the deformed region with $Z \approx 100$ and $N \approx 152$. The strongly downsloping orbitals originating from spherical subshells and active near the predicted shell closures may approach the Fermi surface in these deformed nuclei. The rotational properties of nuclei in this mass region are strongly affected by these spherical orbitals. For example, the $1/2$ [521] and $3/2$ [521] orbitals are of particular interest since they stem from the spherical spin doublets $2f_{7/2}$ and $2f_{5/2}$ orbitals.

Both in-beam spectroscopy and spectroscopy following isomeric states or alpha decays have been used to study nuclei with $Z \approx 100$ [29-32]. These nuclei are well-deformed; for example, the quadrupole deformation parameter $\beta_2 \approx 0.28$ for ^{262}Fm and ^{262}No [33-35]. Many high-spin rotational bands in even-even nuclei (e.g., ^{262}Fm , ^{262}No , ^{262}Cf [36], ^{262}Fm [34], ^{262}No [33, 35]) and odd-A nuclei (e.g., ^{262}Cm and ^{262}Cf [37], ^{263}No [38, 39], ^{264}Md [40], ^{264}Lr [41]) have been established in recent years. The study of these nuclei is certainly also very interesting in itself. The rotational spectra in these nuclei can reveal detailed information on single-particle configurations, shell structure, stability against rotation, high-K isomerism, etc.

Theoretically, deformations, shell structure, rotational properties, and high-K isomeric states have been studied using self-consistent mean-field models [42-45], macroscopic-microscopic models [45-51], the projected shell model [52-54], cranked shell models [55-57], the quasiparticle (qp) phonon model [58], the particle-triaxial-rotor model [59], the heavy shell model [60], etc. Continuing from a recently published Rapid Communication [57], in this work we present results of a systematic study of the single-particle structure and rotational properties of nuclei with $Z \approx 100$. The cranked shell model (CSM) with pairing correlations treated by a particle-number conserving (PNC) method [61, 62] is used. In contrast to the conventional Bardeen-Cooper-Schrieffer (BCS) or Hartree-Fock-Bogolyubov (HFB) approach, in the PNC method the Hamiltonian is solved directly in a truncated Fock space [63]. Thus particle number is conserved and Pauli blocking effects are taken into account exactly. Note that the PNC scheme has been implemented both in relativistic and nonrelativistic mean-field models [64, 65], in which single-particle states are calculated from self-consistent mean-field potentials instead of the Nilsson potential.

The paper is organized as follows. A brief introduction to the PNC treatment of pairing correlations within the CSM and applications of the PNC-CSM are presented in Section II. Numerical details, including a new set of Nilsson parameters (ϵ, μ), deformation parameters, and pairing parameters are given in Section III. PNC-CSM calculation results for even-even, odd-A, and odd-odd nuclei are presented in Section IV. A brief summary is given in Section V.

Theoretical Framework

The cranked Nilsson Hamiltonian of an axially symmetric nucleus in the rotating frame reads [62, 66]

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

where H_{Nil} is the Nilsson Hamiltonian [4], $-\omega J_x$ is the Coriolis interaction with cranking frequency ω about the x-axis (perpendicular to the nuclear symmetry z-axis). $H_P = H_P^{(0)} + H_P^{(2)}$ is the pairing interaction:

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

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

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 common shell-model calculations, a cranked many-particle configuration (CMPC) truncation (Fock space truncation) is adopted, which is crucial to make the PNC calculations for low-lying excited states both workable and sufficiently accurate [63, 67]. 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, sufficiently accurate solutions for low-lying excited eigenstates are obtained.

The angular momentum alignment of $|\psi\rangle$ can be separated into diagonal and off-diagonal parts:

$$\langle \psi | J_x | \psi \rangle = \sum_i C_i^2 \langle i | J_x | i \rangle + 2 \sum_{i < j} C_i C_j \langle i | J_x | j \rangle,$$

and the kinematic moment of inertia (MOI) of $|\psi\rangle$ is

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

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 [62, 68]. After a certain permutation of creation operators, $|i\rangle$ and $|j\rangle$ can be recast into

$$|i\rangle = (-1)^{M_{i\mu}}|\mu\dots\rangle, \quad |j\rangle = (-1)^{M_{j\nu}}|\nu\dots\rangle,$$

where the ellipsis stands for the same particle occupation, and $(-1)^{M_{i\mu}} = \pm 1$, $(-1)^{M_{j\nu}} = \pm 1$ according to whether the permutation is even or odd. Therefore, the kinematic MOI of $|\psi\rangle$ can be written as

$$J^{(1)} = \sum_{\mu} n_{\mu} j_x(\mu) + \sum_{\mu \neq \nu} n_{\mu\nu} j_x(\mu\nu),$$

where

$$n_{\mu} = \sum_i |C_i|^2 P_{i\mu}$$

is the occupation probability of the cranked orbital $|\mu\rangle$, $P_{i\mu} = 1$ if $|\mu\rangle$ is occupied in $|i\rangle$, and $P_{i\mu} = 0$ otherwise.

We note that because $R_x(\pi) = e^{-i\pi J_x}$, $[J_x, J_z] \neq 0$, the signature scheme breaks the quantum number K . However, it has been pointed out that [62, 69], although $[J_x, J_z] \neq 0$, $[R_x(\pi), J_z^2] = 0$. Thus we can construct simultaneous eigenstates of $(R_x(\pi), J_z^2)$. Each CMPC $|i\rangle$ is chosen as a simultaneous eigenstate of (H_0, J_z^2) .

It should be noted that, though the projection K of the total angular momentum of a deformed spheroidal nucleus is a constant of motion, K cannot remain constant when the rotational frequency ω is non-zero due to the Coriolis interaction. However, in the low- ω region, K may serve as a useful quantum number characterizing a low-lying excited rotational band.

The PNC-CSM treatment has been used successfully to describe high-spin states of normally deformed nuclei in the rare-earth and actinide regions, and superdeformed nuclei in the $A \approx 190$ region. Multi-quasiparticle high- K isomer states have been investigated in detail in well-deformed Lu ($Z = 71$), Hf ($Z = 72$), and Ta ($Z = 73$) isotopes [70, 71]. Backbendings in Yb ($Z = 70$) and Tm ($Z = 68$) isotopes are clearly understood, especially the occurrence of sharp backbending in some nuclei [72, 73]. Upbending mechanisms in the actinide nuclei ${}^21\text{Md}$ and ${}^23\text{No}$ have also been analyzed [56].

In superdeformed nuclei around the $A \approx 190$ region, the effects of quadrupole pairing on the downturn of dynamic MOIs have been analyzed [66], and the evolution of dynamic MOIs and alignment additivity arising from interference terms have been investigated [74].

Some general features in nuclear structure physics have also been well explained in the PNC-CSM scheme, e.g., large fluctuations of odd-even differences in MOIs [68], nonadditivity in MOIs [75], the microscopic mechanism of identical bands in normally deformed and superdeformed nuclei [76, 77], and the nonexistence of pairing phase transition [78]. In Ref. [57], high-spin rotational bands in ${}^2, {}^2$ Cm and 2 Cf established in Ref. [37] were calculated using the PNC-CSM method and upbending mechanisms were discussed. This paper is an extension of [57], providing more details and a systematic investigation of nuclei with $Z \approx 100$.

Numerical Details

A. A New Set of Nilsson Parameters

The Nilsson parameters κ and μ proposed for nuclei with $Z \approx 100$, which were given in Ref. [57], are shown in Table I. Note that the readjustment of Nilsson parameters is also necessary in some other mass regions of the nuclear chart [80–82], and the l -dependence was already included in Refs. [80, 81].

The conventional Nilsson parameters (κ, μ) proposed in Refs. [4, 79] are optimized to reproduce experimental level schemes for rare-earth and actinide nuclei. However, these parameter sets cannot describe well the experimental level schemes of nuclei studied in this work. By fitting the experimental single-particle levels in odd- A nuclei with $Z \approx 100$, we obtained a new set of Nilsson parameters (κ, μ) that depend on the main oscillator quantum number N as well as the orbital angular momentum l [57].

B. Deformation Parameters

There are not enough experimental values of deformation parameters for the very heavy nuclei with $Z \approx 100$. According to available data, the quadrupole deformation parameter $\beta_2 \approx 0.28 \pm 0.02$ for 2 Fm [34] and ${}^2, {}^2$ No [35]. The values used in various calculations or predicted by different models differ significantly. Figure 1 [Figure 1: see original paper] shows the experimental quadrupole deformations (pink stars) and those predicted by macroscopic-microscopic (MM) models [46, 48] (blue triangles) and the finite-range droplet model (FRDM) [11] (red solid circles). The deformation parameters from the two MM models [46, 48] are very close, so we show only the results from Ref. [48]. Figure 1 shows that the deformation parameters from MM and FRDM models do not agree with experimental values, especially those from FRDM. Both experimental and predicted values indicate that deformations reach a maximum at 2 No ($Z = 102$ and $N = 152$), which partly guides our choice of deformation parameters.

The deformations are input parameters in the PNC-CSM calculations (black squares in Fig. 1). They are chosen to be close to existing experimental values and to change smoothly with proton and neutron number. The deformation parameters ε_2 and ε_4 used in our PNC-CSM calculations for even-even nuclei with $Z \approx 100$ are listed in Table II. The deformations of odd- A and odd-odd

nuclei are taken as the average of neighboring even-even nuclei. These chosen parameters may have some discrepancy from empirical values, which may lead to deviations in single-particle levels if the levels are very close. For example, the level sequence of the 1-qp bands will change in an isotonic or isotopic chain (e.g., see Figs. 6 and 11) due to deformation staggering in neighboring nuclei. This staggering exists in FRDM, as seen in Fig. 1. Some previous calculations have shown that octupole correlations play important roles in this mass region [53, 83, 84]. In the present work, octupole deformation is not yet included. We note that octupole effects may modify the single-particle level scheme, as will be discussed later for the low excitation energy of the $\nu 5/2^+[622]$ states in $N = 151$ isotones in Sec. IV B.

C. Pairing Strengths and CMPC Space

The effective pairing strengths G_0 and G_2 can be determined from odd-even differences in nuclear binding energies. They are connected with the dimension of the truncated CMPC space. The CMPC space for the heavy nuclei studied in this work is constructed in the proton $N = 4, 5, 6$ shells and neutron $N = 6, 7$ shells. The dimensions of the CMPC space for nuclei with $Z \approx 100$ are about 1000 for both protons and neutrons. The corresponding effective monopole and quadrupole pairing strengths are shown in Table III. Since we are interested only in yrast and low-lying excited states, the number of important CMPCs involved (weight $> 1\%$) is not very large (usually < 20), and almost all CMPCs with weight $> 0.1\%$ are included.

The stability of PNC calculation results against changes in CMPC space dimension has been investigated in Refs. [62, 67, 77]. A larger CMPC space with renormalized pairing strengths gives essentially the same results. The calculated MOIs of the ground-state band (GSB) in ${}^2\text{Cm}$ using different CMPC space dimensions (1000 and 1500) are compared in Fig. 2 [Figure 2: see original paper]. The red dotted line shows results with CMPC space dimensions of about 1500 for both protons and neutrons. The effective pairing strengths used are $G_p = 0.35$ MeV, $G_{2p} = 0.03$ MeV, $G_n = 0.27$ MeV, and $G_{2n} = 0.013$ MeV, which are slightly smaller than those used when CMPC dimensions are about 1000 ($G_p = 0.40$ MeV, $G_{2p} = 0.035$ MeV, $G_n = 0.30$ MeV, and $G_{2n} = 0.020$ MeV, as given in Table III). These two results agree well with each other and both reproduce experiment well, indicating that solutions for low-lying excited states are quite satisfactory.

Results and Discussions

A. Cranked Nilsson Levels

Figure 3 [Figure 3: see original paper] shows calculated cranked Nilsson levels near the Fermi surface of ${}^2\text{Fm}$. 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 protons, the sequence of single-particle levels near the Fermi

surface is exactly the same as that determined from experimental information on ${}^2\text{Es}$ [31]. The sequence of single-neutron levels near the Fermi surface is also very consistent with that determined from experimental information on ${}^2\text{Fm}$ [31], with the only exception being the $\nu 5/2^+[622]$ orbital, which will be discussed in the next subsection.

Figure 3 shows a proton gap at $Z = 100$ and a neutron gap at $N = 152$, consistent with experiment and calculations using a Woods-Saxon potential [85]. The position of the proton orbitals $1/2^- [521]$ and $3/2^- [521]$ is very important because they stem from the spherical spin partners $2f_{5/2,7/2}$ orbitals. The magnitude of spin-orbit splitting of these partners determines whether the next proton magic number is $Z = 114$ or 120 . Note that the cranked relativistic Hartree-Bogolyubov theory has been used to investigate the spin-orbit splitting of these partners in Ref. [42]. The calculated proton levels indicate that the $Z = 120$ gap is large whereas the $Z = 114$ gap is small.

The neutron $1/2^+[620]$ orbital is the highest-lying neutron orbital from above the $N = 164$ spherical subshell ($2g_{7/2}$), on which a high-spin rotational band has been established in ${}^2\text{Cm}$ [37]. This orbital also provides new information for studying states close to the next closed neutron shell.

B. 1-qp Bandhead Energies

First we choose ${}^2\text{Cm}$ as an example to compare theoretical 1-qp bandhead energies with data in Fig. 4 [Figure 4: see original paper]. The calculated results obtained using conventional Nilsson parameters [4] deviate significantly from experimental values. With the modified parameters given in Table I, remarkably good agreement with data is achieved. For comparison, results from the Woods-Saxon (WS) potential [50] are also shown (bandhead energies are taken from Table II of Ref. [50], except that of $7/2^+[613]$, which is taken from Fig. 1 of the same article). Generally speaking, for 1-qp spectra of nuclei with $Z \approx 100$, the Woods-Saxon potential gives better agreement with data. For example, the root-mean-square deviation of theoretical 1-qp bandhead energies from experimental values is about 270 keV for neutrons using modified Nilsson parameters, while this deviation is about 200 keV using the Woods-Saxon potential [50].

Figures 5-12 show experimental and calculated bandhead energies of low-lying 1-qp bands for even- Z and odd- N isotones with $N = 145-153$ (one-quasineutron states) and odd- Z and even- N isotopes with $Z = 97-103$ (one-quasiproton states). In these figures, 1-qp states with energies around or less than 0.8 MeV are shown, and positive- and negative-parity states are denoted by black and red lines, respectively. Generally, agreement between calculation and experiment is satisfactory. Next we discuss these 1-qp states in detail.

$N = 145$ Isotones Experimental and calculated bandhead energies of low-lying one-quasineutron bands for $N = 145$ isotones are compared in Fig. 5 [Figure 5: see original paper]. Data are available only for ${}^2\text{Cm}$ [86] and ${}^2\text{Cf}$

[87], and they are reproduced quite well by theory. The ground state of each $N = 145$ isotone studied is $\nu 1/2^+$ [631]. The energy of $\nu 5/2^+$ [622] steadily decreases with increasing Z in both experimental and calculated spectra. The lowering of $\nu 7/2^+$ [624] with increasing Z is also seen experimentally but is less striking in calculations. In each isotone, a low-lying $\nu 7/2^-$ [743] state is predicted but not observed, consistent with Ref. [50].

$N = 147$ Isotones Low-lying one-quasineutron levels for $N = 147$ isotones ${}^2\text{ }^3\text{Cm}$ [88], ${}^2\text{ Cf}$ [87], and ${}^2\text{ Fm}$ [89] were identified experimentally. Their ground states are $\nu 5/2^+$ [622], $\nu 1/2^+$ [631], and $\nu 7/2^+$ [624], respectively. However, PNC-CSM predicts $\nu 5/2^+$ [622] as the ground state for all these isotones, as seen in Fig. 6 [Figure 6: see original paper]. The same result was obtained recently using a two-center shell model [45]. In our calculations, the energies of these three levels are very close; a small change in deformation parameters would modify their order. This may be one reason for the disagreement in ground-state configuration between theory and experiment. A similar situation occurs in Bk and Es isotopes, where the energies of $\pi 3/2^-$ [521] and $\pi 7/2^+$ [633] are very close and these two 1-qp levels cross at $N = 152$.

$N = 149$ Isotones Low-lying one-quasineutron levels for $N = 149$ isotones ${}^2\text{ Cm}$ [90], ${}^2\text{ Cf}$ [91], ${}^2\text{ Fm}$ [92], and ${}^2\text{ }^1\text{No}$ [89] were identified experimentally. All their ground states are $\nu 7/2^+$ [624]. Comparison with experiment is shown in Fig. 7 [Figure 7: see original paper]. Nearly all 1-qp bandhead energies are well reproduced by PNC-CSM calculations. The energy of $\nu 1/2^+$ [631] is much lower in ${}^2\text{ }^1\text{No}$ than in ${}^2\text{ Cm}$, but in our calculations this level appears almost unchanged with increasing proton number. Our results are very similar to those in Ref. [93]. For each observed level, the energy reaches a maximum in ${}^2\text{ Cf}$, which cannot be reproduced by our calculations.

$N = 151$ Isotones Many theoretical models predict that the first excited state in $N = 151$ isotones should be $\nu 7/2^+$ [624] (see, e.g., Ref. [50]). This is inconsistent with experimental results, which show the first excited state is $\nu 5/2^+$ [622]. The low excitation energy of $\nu 5/2^+$ [622] states in $N = 151$ isotones has been interpreted as a consequence of a low-lying $K^\pi = 2^-$ octupole phonon state [97]. Note that in Ref. [42], using the cranked relativistic Hartree-Bogolyubov theory, the level sequence in $N = 151$ isotones is consistent with experiment, but it cannot reproduce the level sequence in $N = 149$ isotones.

As seen in Fig. 8 [Figure 8: see original paper], the level sequence in most nuclei is consistent with experimental data, with the obvious exception of the $\nu 5/2^+$ [622] orbital. The $\nu 7/2^+$ [624] level observed in ${}^2\text{ }^3\text{No}$ at 355 keV is from Ref. [38]. A recent experiment [39] observed a very similar level scheme that was, however, assigned the $\nu 9/2^-$ [734] configuration. This will be discussed in Sec. IV.

$N = 153$ Isotones Experimental and calculated bandhead energies of low-lying one-quasineutron bands for $N = 153$ isotones are compared in Fig. 9 [Figure 9: see original paper]. One-quasineutron levels for ${}^2\text{Cm}$ [98], ${}^2\text{Cf}$ [99], ${}^2\text{Fm}$ [100], and ${}^2\text{No}$ [101] were identified experimentally. Our calculations predict $\nu 1/2^+$ [620] as the ground state for all these isotones, consistent with data. However, the level order of $\nu 7/2^+$ [613] and $\nu 3/2^+$ [622] from our calculation is inverted compared to data. This also occurs in Ref. [50]. Another problem is that $\nu 11/2^-$ [725] states in all isotones from our calculation are systematically higher than experimental values. In each isotope, a low-lying $\nu 7/2^-$ [743] state is predicted but not observed.

Bk Isotopes Low-lying one-quasiproton levels for Bk ($Z = 97$) isotopes ${}^2\text{Bk}$ [102], ${}^2\text{Bk}$ [103], ${}^2\text{Bk}$ [104], and ${}^2\text{Bk}$ [105] were identified experimentally. Comparison between data and our calculation is shown in Fig. 10 [Figure 10: see original paper]. The two levels $\pi 3/2^-$ [521] and $\pi 7/2^+$ [633] are very close, usually with energy differences less than 50 keV. The ground states are $\pi 3/2^-$ [521] for all Bk isotopes except ${}^2\text{Bk}$. Our calculations predict $\pi 3/2^-$ [521] as the ground state for all Bk isotopes. The deviation in ${}^2\text{Bk}$ may be due to deformation staggering. Nearly all calculated 1-quasiproton energies in Bk isotopes are slightly larger than experimental values.

Es Isotopes Low-lying one-quasiproton levels for Es ($Z = 99$) isotopes ${}^2\text{Es}$, ${}^2\text{Es}$, ${}^2\text{Es}$, ${}^2\text{Es}$, ${}^2\text{Es}$ [106, 107] were identified experimentally. Comparison between data and our calculation is shown in Fig. 11 [Figure 11: see original paper]. The ground states are $\pi 7/2^+$ [633] for all Es isotopes except ${}^2\text{Es}$. Our calculations predict $\pi 7/2^+$ [633] as the ground state for all Es isotopes. The deviation in ${}^2\text{Es}$ may also be due to deformation staggering. Our calculations show that bandhead energies of negative-parity states are all very small (less than 400 keV), consistent with experiment.

Md and Lr Isotopes With increasing proton number, data become increasingly scarce. Figure 12 [Figure 12: see original paper] shows comparison between experimental values and our calculations for Md and Lr isotopes. Data are available only for ${}^2\text{Md}$ [109], ${}^2\text{Md}$ [108], and ${}^2\text{Lr}$ [109], and they are reproduced quite well by theory.

From these discussions, we see that the new Nilsson parameters can satisfactorily describe 1-qp spectra of nuclei with $Z \approx 100$, though some discrepancies remain. Based on our experience, it is quite difficult to improve this situation within the Nilsson model framework. One alternative might be to use the Woods-Saxon potential instead of the Nilsson potential.

C. Even-Even Nuclei

Experimental kinematic MOIs for each band are extracted by

$$J^{(1)}(I) = \frac{2I + 1}{E_\gamma(I + 1 \rightarrow I - 1)}$$

separately for each signature sequence within a rotational band. The relation between rotational frequency ω and angular momentum I is

$$\hbar\omega(I) = \frac{E_\gamma(I + 1 \rightarrow I - 1)}{I_x(I + 1) - I_x(I - 1)},$$

where

$$I_x(I) = \sqrt{(I + 1/2)^2 - K^2},$$

with K being the projection of total nuclear angular momentum along the symmetry axis of an axially symmetric nucleus.

Figure 13 [Figure 13: see original paper] shows experimental and calculated MOIs of GSBs in even-even Cm, Cf, Fm, and No isotopes. Experimental (calculated) MOIs are denoted by solid circles (solid lines). Experimental MOIs of all these GSBs are well reproduced by PNC-CSM calculations. For some nuclei with no data (e.g., ^{242}Cm), we show only PNC-CSM results. Figure 13 shows that with increasing proton number Z in any isotonic chain, upbendings become less pronounced.

It is well known that backbending is caused by crossing of the GSB with a pair-broken band based on high- j intruder orbitals [110], in this mass region the $\pi i_{13/2}$ and $\nu j_{15/2}$ orbitals. However, in several nuclei there is no evidence for $\nu j_{15/2}$ alignment. It has been pointed out in Ref. [57] that 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 off-diagonal parts contribute slightly if the neutron $j_{15/2}$ orbital is not blocked.

To examine upbending more clearly, Fig. 14 [Figure 14: see original paper] shows experimental (solid circles) and calculated (solid lines) alignment $i = \langle J_x \rangle - \omega J_0 - \omega^3 J_1$ for GSBs in $N = 150$ isotones. For other isotones the results are very similar. Upbending frequencies of these GSBs are about 0.20 – 0.25 MeV.

A major advantage of the PNC method is that total particle number $N = \sum_\mu n_\mu$ is exactly conserved, while occupation probability n_μ for each orbital varies with rotational frequency $\hbar\omega$. By examining the ω -dependence of orbitals near the Fermi surface, one can learn how Nilsson levels evolve with rotation and gain insight into upbending mechanisms. Figure 15 [Figure 15: see original paper] shows occupation probability n_μ of each orbital μ (including both $\alpha = \pm 1/2$)

near the Fermi surface for GSBs in $N = 150$ isotones. Top and bottom rows are for protons and neutrons, respectively. Positive (negative) parity levels are denoted by blue solid (red dotted) lines. Orbitals where n_μ changes little (contributing little to upbending) are denoted by black lines. Nilsson levels far above the Fermi surface ($n_\mu \sim 0$) and far below ($n_\mu \sim 2$) are not shown.

Figure 15 shows that the occupation probability of $\pi 7/2^+[633]$ ($\pi i_{13/2}$) drops gradually from 0.5 to nearly zero as cranking frequency $\hbar\omega$ increases from about 0.20 to 0.30 MeV, while occupation probabilities of some other orbitals increase slightly. This can be understood from cranked Nilsson levels in Fig. 3. 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 $\hbar\omega$, it moves further 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 ${}^2\text{Cf}$, but band crossing occurs at $\hbar\omega_c \sim 0.25$ MeV, slightly larger than in ${}^2\text{Cm}$. Thus band crossings in both cases are mainly caused by $\pi i_{13/2}$ orbitals. For ${}^2\text{Fm}$ and ${}^2{}^{2}\text{No}$, occupation probabilities of $\pi i_{13/2}$ orbitals increase slowly as $\hbar\omega$ increases from about 0.20 to 0.30 MeV, so there is no sharp band crossing from proton orbitals.

Focusing on neutron orbitals (bottom row of Fig. 15), the four figures show very similar patterns. With increasing $\hbar\omega$, n_μ of $\nu 7/2^+[624]$ orbitals increases slowly while that of high- Ω (deformation-aligned) $\nu 9/2^- [734]$ orbitals ($j_{15/2}$) decreases slowly. Thus only a small contribution from neutrons to upbending is expected for GSBs in $N = 150$ isotopes. Neutron band-crossing frequencies are about 0.20 – 0.25 MeV, very close to proton band-crossing frequencies, so neutrons and protons from high- j orbits compete strongly in rotation alignment, as pointed out in Ref. [54].

The contribution of each proton (top row) and neutron (bottom row) major shell to angular momentum alignment $\langle J_x \rangle$ for GSBs in $N = 150$ isotones is shown in Fig. 16 [Figure 16: see original paper]. The diagonal $\sum_\mu j_x(\mu)$ and off-diagonal parts $\sum_{\mu < \nu} j_x(\mu\nu)$ in Eq. (5) from proton $N = 6$ and neutron $N = 7$ shells are shown by dashed lines. Note that in this figure, the smoothly increasing part of alignment represented by the Harris formula ($\omega J_0 + \omega^3 J_1$) is not subtracted (cf. caption of Fig. 14). Figure 16 clearly shows that upbendings for GSBs in ${}^2\text{Cm}$ at $\hbar\omega_c \sim 0.20$ MeV and in ${}^2\text{Cf}$ at $\hbar\omega_c \sim 0.25$ MeV mainly come from the proton $N = 6$ shell. Furthermore, upbending in ${}^2\text{Cm}$ comes mainly from the off-diagonal part of the proton $N = 6$ shell, while both diagonal and off-diagonal parts contribute in ${}^2\text{Cf}$. The off-diagonal part of the neutron $N = 7$ shell contributes only a little to upbending.

The situation is very different for ${}^2\text{Fm}$ and ${}^2{}^{2}\text{No}$. For these nuclei, contributions to upbending from off-diagonal parts of both proton $N = 6$ and neutron $N = 7$ shells are nearly equal. This is because with increasing proton number Z , the Fermi surface moves further from the $\pi 7/2^+[633]$ orbital. In this case, the high- j

but high- Ω (deformation-aligned) $\pi 9/2^+[624]$ orbital becomes close to the Fermi surface.

For clearer understanding of the upbending mechanism, Fig. 17 [Figure 17: see original paper] shows contributions of intruder proton orbitals $i_{13/2}$ (top row) and intruder neutron orbitals $j_{15/2}$ (bottom row) to angular momentum alignment $\langle J_x \rangle$. Important diagonal (off-diagonal) parts $j_x(\mu)$ [$j_x(\mu\nu)$] in Eq. (5) are denoted by blue solid (red dotted) lines. Orbitals that have no contribution to upbending (some contribute to steady alignment increase) are denoted by black lines. Near proton Fermi surfaces of ${}^2\text{Cm}$ and ${}^2\text{Cf}$, the proton $i_{13/2}$ orbitals are $\pi 5/2^+[642]$ and $\pi 7/2^+[633]$. Other $\pi i_{13/2}$ parentage orbitals are either fully occupied or fully empty (cf. Fig. 15) and have no contribution to upbending. For ${}^2\text{Cm}$, PNC calculations show that after upbending ($\hbar\omega \geq 0.20$ MeV) the off-diagonal part $j_x(\pi 5/2^+[642]\pi 7/2^+[633])$ changes significantly. Alignment gain after upbending mainly comes from this interference term. For ${}^2\text{Cf}$, main contributions to alignment gain after upbending come from the diagonal part $j_x(\pi 7/2^+[633])$ and off-diagonal part $j_x(\pi 5/2^+[642]\pi 7/2^+[633])$. Again this shows that upbending in both cases is mainly caused by $\pi i_{13/2}$ orbitals. For ${}^2\text{Fm}$ and ${}^2\text{No}$, only the off-diagonal part $j_x(\pi 7/2^+[633]\pi 9/2^+[624])$ contributes slightly to upbending.

The absence of $j_{15/2}$ neutron alignment in nuclei of this mass region can be understood from contributions 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 orbitals contribute no alignment to upbending; only interference terms $j_x(\nu 7/2^- [743]\nu 9/2^- [734])$ contribute slightly. Thus strong competition in rotation alignment between high- j protons and neutrons occurs in ${}^2\text{Fm}$ and ${}^2\text{No}$, consistent with Ref. [54].

D. Odd-A Nuclei

Large fluctuations exist in experimental odd-even differences in MOIs, $\delta J/J$. If a high- j intruder orbital near the Fermi surface is blocked, $\delta J/J$ can be quite large (sometimes $>100\%$). It is very difficult to reproduce such large fluctuations with the conventional BCS method, which predicts $\delta J/J \approx 15\%$ [111]. An advantage of PNC-CSM is that Pauli blocking effects are treated exactly, so odd-even differences in MOIs can be reproduced quite well, as shown for rare-earth nuclei [68]. Two high- j orbitals are involved in the present calculations: $\pi 7/2^+[633]$ ($\pi i_{13/2}$) and $\nu 9/2^- [734]$ ($\nu j_{15/2}$). To demonstrate blocking effects, we study four nuclei and compare calculated odd-even differences in MOIs with data:

$$\frac{J({}^{249}\text{Bk } \pi 7/2^+[633]) - J({}^{248}\text{Cm GSB})}{J({}^{248}\text{Cm GSB})} \approx 54\% (\text{Exp.}), 56\% (\text{Cal.})$$

$$\frac{J(^{253}\text{No } \nu 9/2^- [734]) - J(^{252}\text{No GSB})}{J(^{252}\text{No GSB})} \approx 41\% (\text{Exp.}), 46\% (\text{Cal.})$$

The experimentally observed large odd-even differences in MOIs induced by high- j intruder orbitals are reproduced quite well.

Figure 18 [Figure 18: see original paper] shows experimental and calculated MOIs of GSBs for odd- N Cm, Cf, Fm, and No isotopes ($N = 145$ – 153). Experimental MOIs are denoted by solid squares (signature $\alpha = +1/2$) and open squares (signature $\alpha = -1/2$). Calculated MOIs are denoted by solid lines (signature $\alpha = +1/2$) and dotted lines (signature $\alpha = -1/2$). Experimental MOIs of all these 1-qp bands are well reproduced by PNC-CSM calculations, strongly supporting configuration assignments. GSBs in brackets denote PNC-CSM calculated results not yet observed. Note that pairing strengths used in Ref. [57] differ slightly from those used here because the strengths are considered as an average for all these odd- N nuclei.

In $N = 145$ isotones, our calculations predict significant signature splitting at low rotational frequency ($\hbar\omega < 0.20$ MeV) for the $\nu 1/2^+[631]$ orbital. In $N = 153$ isotones, signature splitting of the $\nu 1/2^+[620]$ orbital is also well reproduced. This is understandable from the behavior of cranked Nilsson orbitals $\nu 1/2^+[631]$ and $\nu 1/2^+[620]$ in Fig. 3. In Ref. [57], upbending mechanisms for high-spin rotational GSBs of $^{2,2}\text{Cm}$ and $^{2,2}\text{Cf}$ observed in Ref. [37] were analyzed.

Figure 19 [Figure 19: see original paper] shows results for excited 1-qp bands observed in odd- A Cm, Cf, and No isotopes. They are all well reproduced by PNC-CSM calculations. It is interesting to note that in an earlier experiment on $^{2,3}\text{No}$, a rotational band was established and assigned the $\nu 7/2^+[624]$ configuration [38]. In a later experiment, a similar rotational band was observed [39] but assigned the $\nu 9/2^- [734]$ configuration. Experimental MOIs extracted from [38] using both configurations can be reproduced by PNC calculations, so our calculations cannot distinguish which assignment is correct.

Figure 20 [Figure 20: see original paper] shows experimental and calculated GSBs of odd- Z nuclei, including Bk, Es, and Md isotopes ($N = 146$ – 154). Data for these odd- Z nuclei are very rare. Most data are well reproduced, except for the $\pi 7/2^+[633]$ band in $^{2,3}\text{Es}$. The MOI of this band seems extremely large, with $J^{(1)} > 120 \hbar^2 \text{MeV}^{-1}$. Our calculations show that $\pi 7/2^+[633]$ has small signature splitting at higher rotational frequencies ($\hbar\omega > 0.10$ MeV).

Figure 21 [Figure 21: see original paper] shows results for excited 1-qp bands observed in odd- Z Bk, Es, and Md isotopes.

In some nuclei, an upbending appears around $\hbar\omega \approx 0.25$ MeV in the $\pi 7/2^+[633]$ (signature $\alpha = 1/2$) band according to PNC calculations (e.g., Bk isotopes). Figure 22 [Figure 22: see original paper] shows occupation probabilities n_μ of each orbital μ near the Fermi surface for the $\pi 7/2^+[633]$ ($\alpha = 1/2$) band in $^{2,3}\text{Bk}$. Top and bottom rows are for protons and neutrons, respectively. It is

clear that occupation probabilities of $\pi 5/2^+[642]$ and $\pi 7/2^+[633]$ orbitals drop sharply at $\hbar\omega \approx 0.25$ MeV, while n_μ of $\pi 3/2^- [521]$ increases sharply. Occupation probabilities of neutron orbitals change slowly with increasing $\hbar\omega$, indicating little contribution to upbending.

Figure 23 [Figure 23: see original paper] shows contributions of each proton (top row) and neutron (bottom row) major shell to angular momentum alignment $\langle J_x \rangle$ for the $\pi 7/2^+[633]$ ($\alpha = 1/2$) band in 2 Bk. Diagonal $\sum_\mu j_x(\mu)$ and off-diagonal parts $\sum_{\mu < \nu} j_x(\mu\nu)$ in Eq. (5) from proton $N = 6$ and neutron $N = 7$ shells are shown by dashed lines. Both diagonal and off-diagonal parts from the proton $N = 6$ shell contribute to upbending. PNC calculations show that upbending comes from diagonal parts $j_x(\pi 5/2^+[642])$ and $j_x(\pi 7/2^+[633])$, and off-diagonal parts $j_x(\pi 5/2^+[642]\pi 7/2^+[633])$ and $j_x(\pi 7/2^+[633]\pi 9/2^+[624])$.

E. Odd-Odd Nuclei

When an unpaired proton and neutron in a deformed odd-odd nucleus are coupled, the projections of their total angular momentum on the nuclear symmetry axis, Ω_p and Ω_n , produce two states with $K_> = |\Omega_p + \Omega_n|$ and $K_< = |\Omega_p - \Omega_n|$. They follow the Gallagher-Moszkowski (GM) coupling rules [113]:

$$K_> = |\Omega_p + \Omega_n|, \quad \text{if } \Omega_p = \Lambda_p \pm \frac{1}{2} \text{ and } \Omega_n = \Lambda_n \pm \frac{1}{2}$$

$$K_< = |\Omega_p - \Omega_n|, \quad \text{if } \Omega_p = \Lambda_p \pm \frac{1}{2} \text{ and } \Omega_n = \Lambda_n \mp \frac{1}{2}$$

Rotational bands in odd-odd nuclei in the transfermium region are very rare. The most recent experiment is on 2 Bk [112], where energy splittings between parallel and antiparallel coupled neutron and proton states were measured for six pairs of states. Because residual proton-neutron interaction is not included in our calculations, energies of 2-qp bands in odd-odd nuclei are sums of quasiproton and quasineutron energies; that is, there is no energy splitting between parallel and antiparallel coupling states.

Figure 24 [Figure 24: see original paper] shows experimental and calculated MOIs of 2 Bk. The energy of neutron orbital $\nu 1/2^- [750]$ is too high in our calculation, so we do not consider the $K^\pi = 3^-, 4^- (\pi 7/2^+[633] \otimes \nu 1/2^- [750])$ bands observed in Ref. [112]. Up (down) triangles denote experimental values of $K_>$ ($K_<$) bands. Filled (open) triangles denote signature $\alpha = 0$ (1) bands. Solid (dotted) lines denote calculated results for signature $\alpha = 0$ (1) bands. Most data are reproduced quite well. Calculated MOIs are slightly smaller for $K^\pi = 2^+, 5^+$ bands than experimental values, but much larger for the $K^\pi = 1^-$ band.

MOIs of $K_>$ and corresponding $K_<$ bands are usually the same. However, MOIs of the $K^\pi = 3^+$ band are much larger than those of the $K^\pi = 4^+$ band. This is because for the $K^\pi = 3^+$ band the neutron component is $\nu 1/2^+[620]$ ($\alpha = +1/2$),

whereas for the $K^\pi = 4^+$ band it is $\nu 1/2^+[620]$ ($\alpha = -1/2$), and signature splitting of $\nu 1/2^+[620]$ is very large. Calculated results are very close to data. Similarly, our calculation predicts that this signature splitting results in a large difference between MOIs of $K^\pi = 1^-$ and 2^- bands. However, this is not observed experimentally. When one nucleon is in an $\Omega = 1/2$ orbital, the GM doublet has $\Delta K = 1$, so the two bands are expected to be Coriolis-mixed. This effect can be significant in the $K_<$ band, as identified in odd-odd rare-earth nuclei [114, 115]. Similar MOIs in $K^\pi = 1^-$ and 2^- bands may result from this mixing and need further exploration both experimentally and theoretically.

Summary

In summary, rotational bands in the $A \approx 250$ mass region are investigated using a cranked shell model (CSM) with pairing correlations treated by a particle-number conserving (PNC) method. In the PNC method for pairing correlations, blocking effects are taken into account exactly. By fitting experimental single-particle spectra in these nuclei, a new set of Nilsson parameters (κ and μ) and deformation parameters (ε_2 and ε_4) are proposed. Bandhead energies of 1-qp states below 0.8 MeV are reproduced satisfactorily. Experimentally observed ω variations of MOIs for even-even, odd-A, and odd-odd nuclei are reproduced very well by PNC-CSM calculations. By analyzing the ω -dependence of occupation probabilities of cranked Nilsson orbitals near the Fermi surface and contributions of valence orbitals in each major shell to angular momentum alignment, the upbending mechanism in this region is clearly understood. For Cm and Cf isotopes, upbending in GSBs is mainly caused by intruder proton ($N = 6$) $\pi i_{13/2}$ orbitals. For Fm and No isotopes, neutrons and protons from high- j orbits compete strongly in rotation alignment. The 2-qp states in odd-odd nucleus ${}^2\text{Bk}$ are analyzed in detail.

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