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Structures of Odd Mass Transfermium Nuclei by a Particle-Number Conserving Cranked Shell Model

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Abstract. The cranked-shell model (CSM) with pairing correlations treated by a particle-number conserving (PNC) method is used to study the rotational properties of odd mass transfermium nuclei. In the PNC method, the particle number is conserved and the Pauli blocking effects are taken into account exactly. By fitting the experimental single-particle spectra in these nuclei, a new set of Nilsson parameters (κ and μ) are proposed. The experimental kinematic moments of inertia in these transfermium nuclei are reproduced quite well by the PNC-CSM calculations. The structures of the single-particle states, deformation, high-j intruder orbital and the rotational properties in these nuclei are investigated in detail.

1 Introduction

Since the importance of shell effects on the stability of superheavy nuclei (SHN) was illustrated and the existence of an island of stability of SHN was predicted around Z = 114 and N = 184 [1–5], a lot of efforts have focused on the exploration of SHN. Great experimental progress has been made in synthesizing the superheavy elements. Up to now, superheavy elements with $Z \leq 118$ have been synthesized via cold and hot fusion reactions [6–8]. However, due to the extremely low production cross-sections, these experiments can rarely reveal the detailed spectroscopic information. One indirect way is to study lighter nuclei in the deformed region with $Z \approx 100$ and $N \approx 152$, which are the heaviest systems accessible in present in-beam experiments (see Refs. [9–11] and references therein). The strongly downsloping orbitals originating from the spherical subshells active in the vicinity of the predicted shell closures come close to the Fermi surface of transfermium nuclei due to deformation effect. The rotational properties of transfermium nuclei will be strongly affected by these spherical orbitals. The proton $1/2^-[521]$ orbital is of particular interest since it stems from the spherical $2f_{5/2}$ orbital. The spin−orbit interaction strength of $2f_{5/2} - 2f_{7/2}$ partner governs the size of the possible $Z = 114$ shell gap. Most direct information on the single particle structure of nuclei comes from odd-A nuclei. The first in-beam study of an odd-A nucleus in transfermium nuclei region was the investigation of ^{253}No [12]. Later, in-beam study of rotational state in ^{251}Md was also carried out [13]. The Cranked Shell Model (CSM) with the pairing correlations treated by a Particle-Number Conserving (PNC) method [14,15] is used to study the rotational and single-particle properties of odd mass transfermium nuclei.

2 Theoretical Framework

The Cranked Shell Model Hamiltonian of an axially symmetric nucleus in the rotating frame is expressed as:

$$H_{\rm CSM} = H_0 + H_{\rm P} = \sum_n (h_{\rm Nil} - \omega j_x)_n + H_{\rm P}(0) + H_{\rm P}(2) \ , \tag{1}$$

where $h_{\rm Nil}$ is the Nilsson Hamiltonian [18], $-\omega j_x$ is the Coriolis force with the cranking frequency ω about the x axis (perpendicular to the nuclear symmetry z axis). $H_{\rm P}$ is the pairing including monopole and quadrupole pairing correlations,

$$H_{\rm P}(0) = -G_0 \sum_{\xi\eta} a^\dagger_\xi a^\dagger_{\overline{\xi}} a_{\overline{\eta}} a_\eta \ , \tag{2}$$

$$H_{\rm P}(2) = -G_2 \sum_{\xi\eta} q_2(\xi) q_2(\eta) a^\dagger_\xi a^\dagger_{\overline{\xi}} a_{\overline{\eta}} a_\eta \ , \tag{3}$$

with $\overline{\xi}$ and $\overline{\eta}$ being the time-reversal states of a Nilsson state ξ and η, respectively. The quantity $q_2(\xi) = \sqrt{16\pi/5}\,\langle\xi|\, r^2 Y_{20}\,|\xi\rangle$ 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.

In our calculation, $h_0(\omega) = h_{\rm Nil} - \omega j_x$ is diagonalized firstly to obtain the cranked Nilsson orbitals. Then, $H_{\rm CSM}$ is diagonalized in a sufficiently large Cranked Many-Particle Configuration (CMPC) space to obtain the yrast and low-lying eigenstates. Instead of the usual single-particle level truncation in common shell-model calculations, a cranked many-particle configuration truncation (Fock space truncation) is adopted which is crucial to make the PNC calculations for low-lying excited states both workable and sufficiently accurate [16, 17] . The eigenstate of $H_{\rm CSM}$ is expressed as:

$$|\psi\rangle = \sum_i C_i\,|i\rangle \ , \tag{4}$$

where $|i\rangle$ denotes an occupation of particles in the cranked Nilsson orbitals and C_i is the corresponding probability amplitude. The occupation probability of the cranked orbital μ (including both signature $\alpha = \pm 1/2$) is:

$$\begin{aligned} n_\mu &= \sum_i |C_i|^2 P_{i\mu}, \\ P_{i\mu} &= \begin{cases} 1, & |\mu\rangle \text{ is occupied in CMPC } |i\rangle, \\ 0, & \text{otherwise.} \end{cases} \end{aligned} \tag{5}$$

The angular momentum alignment $\langle J_x \rangle$ of the state $|\psi\rangle$ is given by:

$$\langle\psi| J_x |\psi\rangle = \sum_i |C_i|^2 \langle i| J_x |i\rangle + 2\sum_{i<j} C_i^* C_j \langle i| J_x |j\rangle . \tag{6}$$

Because j_x is an one-body operator, $\langle i|j_x|j\rangle (i \neq j)$ does not vanish only when $|i\rangle$ and $|j\rangle$ differ by one particle occupation. After a certain permutation of creation operators, $|i\rangle$ and $|j\rangle$ are expressed as:

$$|i\rangle = (-)^{M_{i\mu}} |\mu \cdots\rangle, \qquad |j\rangle = (-)^{M_{j\nu}} |\nu \cdots\rangle, \tag{7}$$

where the ellipsis stands for the same particle occupation, and $(-)^{M_{i\mu}} = \pm 1$, $(-)^{M_{i\nu}} = \pm 1$ depend on whether the permutation is even or odd. Then,

$$\begin{aligned} \langle J_x \rangle &= \sum_\mu j_x(\mu) + \sum_{\mu<\nu} j_x(\mu\nu), \qquad (8) \\ j_x(\mu) &= \langle\mu| j_x |\mu\rangle n_\mu, \\ j_x(\mu\nu) &= 2\langle\mu| j_x |\nu\rangle \sum_{i<j} (-)^{M_{i\mu}+M_{j\nu}} C_i^* C_j, \ \ (\mu \neq \nu). \end{aligned}$$

where $j_x(\mu)$ is the direct contribution to $\langle J_x \rangle$ from a particle occupying the cranked orbital μ, and $j_x(\mu\nu)$ is the contribution to $\langle J_x \rangle$ from the interference between two particles occupying the cranked orbitals μ and ν. The kinematic moment of inertia is $\Im^{(1)} = \langle\psi| J_x |\psi\rangle /\omega$.

3 Results and Discussions

The Nilsson parameters (κ, μ) proposed in Refs. [18, 19] cannot well describe the experimental level schemes of transfermium nuclei while it is optimized to reproduce the experimental level schemes for the rare-earth and actinide nuclei. By fitting the experimental single-particle levels in the odd-A nuclei with $Z \approx 100$, we obtained a new set of Nilsson parameters κ and μ (see Table 1) which are dependent on the main oscillator quantum number N as well as on the orbital angular momentum l [20, 22]. The CMPC space in the work of Ref. [20] is constructed in the proton $N = 4, 5, 6$ shells and the neutron $N = 6, 7$ shells. The dimensions of the CMPC space for the nuclei with $Z \approx 100$ are about 1000 both for protons and neutrons.

Table 1. Nilsson parameters κ and μ proposed for the nuclei with $Z \approx 100$.

N	l	κ_p	μ_p	N	l	κ_n	μ_n
4	0,2,4	0.0670	0.654				
5	1	0.0250	0.710	6	0	0.1600	0.320
	3	0.0570	0.800		2	0.0640	0.200
	5	0.0570	0.710		4,6	0.0680	0.260
6	0,2,4,6	0.0570	0.654	7	1,3,5,7	0.0634	0.318

Figure 1 gives the experimental and calculated moments of inertia of excited 1-qp bands in the odd-Z Bk, Es, and Md isotopes. The data are well reproduced by the PNC-CSM calculations. The absence of a signature partner band suggests that the observed rotational band in ^{251}Md is built on the $1/2^-[521]$ Nilsson state. A ground-state spin and parity of $7/2^-$ have been suggested to ^{251}Md [21]. We calculated $J^{(1)}$'s for two signature partner bands which vary smoothly with frequency in ^{251}Md. In order to investigate the effect of the proton $N = 7$ shell on the rotational properties of the transfermium nuclei, the proton $N = 7$

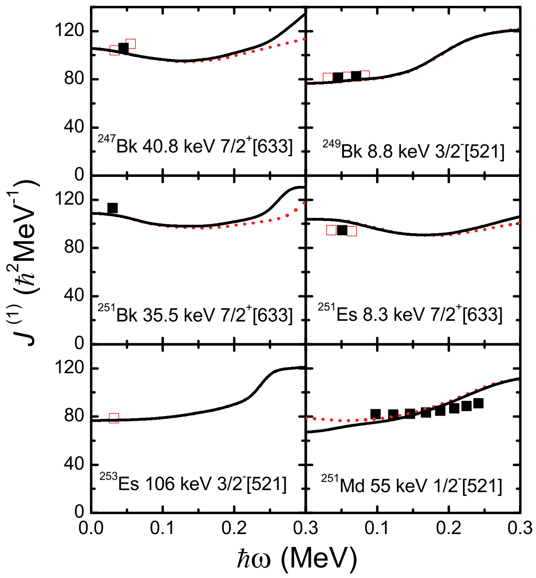

Figure 1. The experimental and calculated MOI's $J^{(1)}$ of the excited 1-qp bands in odd-Z Bk, Es, and Md isotopes. The data are taken from Refs. [10,11] and references therein. The experimental MOI's are denoted by full squares (signature $\alpha = +1/2$) and open squares (signature $\alpha = -1/2$), respectively. The calculated MOI's by the PNC method are denoted by solid lines (signature $\alpha = +1/2$) and dotted lines (signature $\alpha = -1/2$), respectively. The effective pairing interaction strengths for both protons and neutrons for all these odd-N nuclei are, $G_n = 0.30$ MeV, $G_{2n} = 0.02$ MeV, $G_p = 0.25$ MeV, and $G_{2p} = 0.01$ MeV.

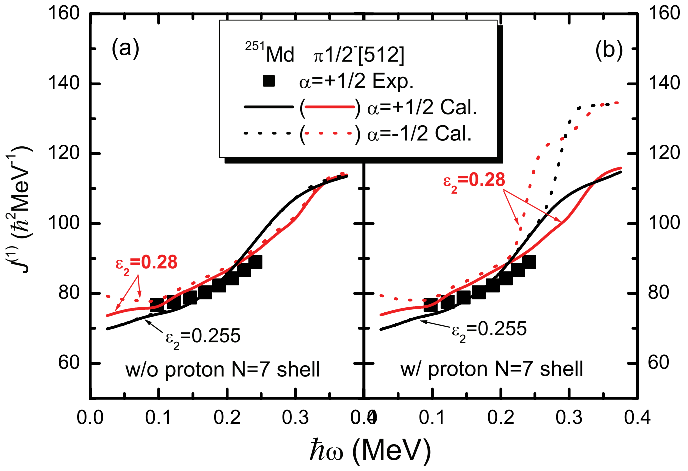

Figure 2. Experimental and calculated kinematic moment of inertia $J^{(1)}$ of the $\pi 1/2^-[521]$ band in ^{251}Md. The experimentally observed $1/2^-[521](\alpha = +1/2)$ band is denoted by solid square. The calculated $J^{(1)}$ are denoted by solid ($\alpha = +1/2$) and dashed lines ($\alpha = -1/2$), respectively. The calculated $J^{(1)}$ for $\varepsilon_2 = 0.28$ and $\varepsilon_2 = 0.255$ are denoted by red and black lines, respectively.

shell is included to construct the CMPC space [23, 24]. Figure 2 shows the experimental and calculated kinematic moment of inertia $J^{(1)}$ of the $1/2^-[521]$ band in ^{251}Md. We find that the $1/2^-[770]$ orbital plays an important role in the rotational properties of ^{251}Md. Since the position of the $1/2^-[770]$ orbital is very sensitive to the deformation [25], we calculate ^{251}Md for $\varepsilon_2 = 0.28$ and 0.255 with and without the proton $N = 7$ shell, respectively [24]. There is no signature splitting when the proton $N = 7$ shell is not included [see Figure 2 (a)]. When the effect of the proton $N = 7$ shell is considered, the signature splitting occurs at $\hbar\omega \approx 0.225$ for $\varepsilon_2 = 0.28$ and $\hbar\omega \approx 0.275$ for $\varepsilon_2 = 0.255$, respectively [see Figure 2 (b)]. When $\varepsilon_2 = 0.28$, a sharp backbending of the $\alpha = -1/2$ band is shown at $\hbar\omega \approx 0.225$MeV while the $\alpha = +1/2$ bands varies smoothly in the whole observed frequency range. The backbending of the $\alpha = -1/2$ band is due to the band crossing between the $1/2^-[521](\alpha = -1/2)$ and $1/2^-[770](\alpha = -1/2)$ configurations at $\hbar\omega \approx 0.255$ MeV. The similar situation is hold for $\varepsilon_2 = 0.255$, but the band crossing occurs at higher frequency $\hbar\omega \approx 0.275$ MeV.

Figure 3 shows the results of excited 1-qp bands observed in the odd-A Cm, Cf, Fm, and No isotopes. They are all well reproduced by the PNC-CSM calculation. In experiment [12], a rotational band has been established and the configuration was assigned as $\nu 7/2 + [624]$ for ^{253}No. In a latter experiment, a similar rotational band has been observed [26], but the configuration was assigned as $\nu 9/2[734]$. In Figure3, when $\varepsilon_2 = 0.258$ for ^{253}No, we can see that

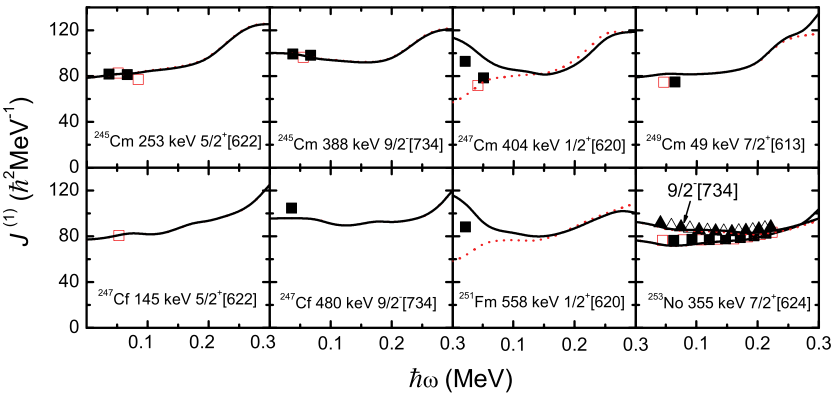

Figure 3. The same as Fig. 18, but for the excited 1-qp bands in odd-N Cm, Cf, and No isotopes.

the experimental MOIs extracted from [12] using these two configurations can be reproduced by the PNC calculations. When ε_2 is taken as 0.29 (see Figure 4), there is a signature splitting for the $9/2^-$ band in PNC calculation while the sig-

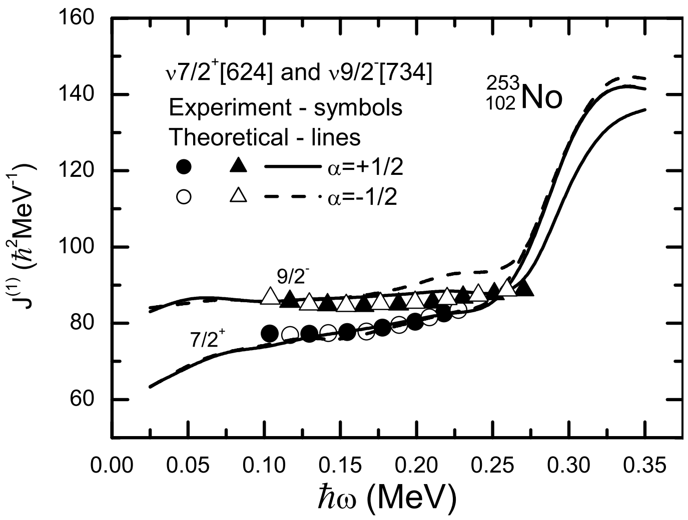

Figure 4. Experimental and theoretical kinematic moment of inertia $J^{(1)}$ for the $\nu 7/2^+[624]$ and $\nu 9/2^+[734]$ bands in ^{253}No. The experimental observed $J^{(1)}$ for $\alpha = +1/2$ and $\alpha = -1/2$ bands of $7/2^+[624](9/2^-[734])$ are denoted by solid and open circles (triangles), respectively. Solid and dashed lines are used for the calculated $J^{(1)}$ for $\alpha = +1/2$ and $\alpha = -1/2$ bands, respectively.

nature splitting is not shown by the experimental data. The calculated splitting of $J^{(1)}$ at $\hbar\omega > 0.20$ MeV is governed by the band crossing between the $9/2[734]$ and $1/2[761]$ configurations. The position of the $1/2[761]$ state is very sensitive to deformation [25]. If the deformation parameter is changed slightly, the splitting would disappear in the experimentally observed frequency range. For example, if $\varepsilon_2 = 0.28$ the band crossing would take place at $\hbar\omega \approx 0.25$ MeV. Therefore, we look forward to the future experiment in which the deformation parameter can be suggested.

4 Conclusion

The rotational bands in the odd mass transfermuim nuclei are investigated by the Cranked Shell Model (CSM) with the pairing correlations treated by a Particle-Number Conserving (PNC) method. In the PNC-CSM method, the blocking effects are taken into account exactly. By fitting the experimental single-particle spectra in these nuclei, a new set of Nilsson parameters (κ and μ) is proposed. The experimentally observed variations of moment of inertia for these nuclei with the frequency ω are reproduced very well by the PNC-CSM calculations. The high-j intruder proton orbital $\pi 1j_{15/2}$ ($1/2^-[770]$) plays an important role in the sharp backbending of the $1/2^-[521](\alpha = -1/2)$ band for ^{251}Md. The neutron high-j orbital $\nu 1/2^-[761]$ is important to the rotational properties in ^{253}No. However, both orbitals of $\pi 1/2^-[770]$ and $\nu 1/2^-[761]$ are very sensitive to the deformation. Therefore, to understand the properties of these high-j orbital, it is necessary to study the deformation of tranfermium nuclei in detail in the future.

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