# Ground-state properties of rare-earth nuclei in the Nilsson mean-field plus extended-pairing model

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The Nilsson mean-field plus extended-pairing model for deformed nuclei is applied to describe the ground-state properties of selected rare-earth nuclei. Binding energies, even-odd mass differences, energies of the first pairing excitation states, and moments of inertia for the ground-state band of  $^{152-164}$ Er,  $^{154-166}$ Yb, and  $^{156-168}$ Hf are calculated systematically in the model employing both proton-proton and neutron-neutron pairing interactions. The pairing interaction strengths are determined as a function of the mass number in the isotopic chains. In comparison with the corresponding experimental data, it is shown that pairing interaction is crucial in elucidating the properties of both the ground state and the first pairing excitation state of these rare-earth nuclei. With model parameters determined by fitting the energies of these states, ground-state occupation probabilities of valence nucleon pairs with angular momentum J = 0, 1, ..., 12 for even-even  $^{156-162}$ Yb are calculated. It is inferred that the occupation probabilities of valence nucleon pairs with odd angular momenta. The results clearly indicate that *S*, *D*, and *G* valence nucleon pairs dominate in the ground state of these nuclei.

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## I. INTRODUCTION

Nuclear pairing correlations, as an important part of the residual interactions necessary to augment any nuclear meanfield theory, represent one of the main and longstanding pillars of current understanding of nuclear structure [1]. For example, the pairing interaction of the nuclear shell model plays a key role in reproducing ground-state and low-energy spectroscopic properties of nuclei, such as binding energies, odd-even effects, single-particle occupancies, excitation spectra, moments of inertia, etc. [2-4]. Bohr, Mottelson, Pines, and Belyaev were the first to introduce the Bardeen-Cooper-Schrieffer (BCS) theory for superconductivity in condensed matter [5] to descriptions of pairing phenomena in nuclei [2,6], which provides a simple yet clear picture that demonstrates the importance of the pairing interaction in nuclei. However, as an approximate theory, both the BCS and the more refined Hartree-Fock-Bogolyubov (HFB) methods suffer from serious drawbacks in nuclei due to the fact that the number of valence nucleons under the influence of the pairing force is too few to be treated by such particlenumber nonconserved (quasiparticle) approximations. A remedy in terms of particle-number projection complicates the algorithms considerably, often without yielding a better description of higher-lying excited states that are a natural part of the spectrum of the pairing Hamiltonian [7–9]. Alternatively, shell model calculations provide successful descriptions but face a combinatorial growth of model space sizes, and hence, for heavy nuclei, truncation schemes are normally needed and applicability is often limited by existing computer resources. The projected shell model (PSM) provides a way to overcome this difficulty [10]. By using the PSM scheme, it is shown that the projected BCS vacuum for a well-deformed system is very close to the SU(3) dynamical symmetry limit of an S-D pair fermion system [11]. On the other hand, the tremendous success of the interacting boson model (IBM) [12] suggests that *s* and *d* pairs play a dominant role in the spectroscopy of low-lying excitations [13,14]. It is shown that, by using the exact solutions of the standard pairing model (Richardson-Gaudin method [15]), the angular momentum distributions of the Richardson pairs in the ground state of the deformed <sup>174</sup>Yb nucleus can be used to clarify the microscopic foundation of the IBM; these distributions, however, are strikingly different from the ones obtained in the BCS ground state [16].

More recently, the Nilsson mean-field plus extendedpairing model has been proposed to describe deformed nuclei [17], which includes pairing interactions among valence pairs in different orbits up to infinite order. It has been shown in our recent work that the extended pairing model can be regarded as the standard pairing Hamiltonian at a first-order approximation; namely, only the lowest energy eigenstate described by the Racah quasispin formulism of the standard pure pairing interaction part is taken into consideration, and the results thus display pair structures similar to the ones found in the low-lying states of the standard pairing model [18]. The advantage of the model lies in the fact that it can be solved more easily than the standard pairing model. Though solutions of the standard pairing model can now be obtained more easily by using the extended Heine-Stieltjes polynomial approach [19], the extended pairing model has been proved to be more efficient, especially when both the number of valence nucleon pairs and the number of single-particle orbits are large, which, therefore, is more suitable to be used for rare-earth nuclei [20]. While so far the calculations for rare-earth nuclei employ a frozen-pair approximation [20], a more realistic approach for systematically understanding the ground-state properties has yet to be developed.

In this paper, we use the Nilsson mean-field plus extendedpairing model with both proton-proton and neutron-neutron pairing interactions to investigate Er, Yb, and Hf isotopes in the rare-earth region. Binding energies, even-odd mass differences, energies of the first pairing excitation states and the moments of inertia of these nuclei are calculated. The results indicate that the extended pairing model is helpful to understand the structural properties of these deformed nuclei in the low-energy regime. We especially focus on analyzing the ground-state occupation probabilities of valence nucleon pairs with various angular momentum quantum numbers (J = 0, 1, ..., 12) for even-even nuclei. We study which pairs—in terms of their J angular momentum—are important in the ground state and whether S and D pairs indeed dominate in the ground state of these nuclei, as implied in the IBM. Moreover, we intend to provide a reasonable range of pair interaction strength in the model by comparing our model calculations with the corresponding experimental data.

#### **II. THE EXTENDED PAIRING MODEL**

The Nilsson mean-field plus standard-pairing Hamiltonian for a deformed nucleus is given by

$$\hat{H} = \sum_{j=1}^{p} \epsilon_{j} n_{j} - G_{st} \sum_{i,j=1}^{p} b_{i}^{\dagger} b_{j}, \qquad (1)$$

where *p* is the total number of Nilsson levels (orbits) considered,  $G_{st} > 0$  is the overall pairing strength,  $\epsilon_j$  are the single-particle energies obtained in the Nilsson model,  $n_j = a_{j\Omega_j}^{\dagger}a_{j\Omega_j} + a_{j\bar{\Omega}_j}^{\dagger}a_{j\bar{\Omega}_j}$  is the fermion number operator for the *j*th Nilsson level, and  $b_i^{\dagger} = a_{i\Omega_i}^{\dagger}a_{i\bar{\Omega}_i}[b_i = (b_i^{\dagger})^{\dagger} = a_{i\bar{\Omega}_i}a_{i\Omega_i}]$  are pair creation [annihilation] operators, where  $\Omega_i$  is the quantum number of the third component of the total angular momentum in the intrinsic frame for the *i*th Nilsson single-particle state, while  $\bar{\Omega}_i$  denotes the time reversal state. The Hamiltonian of the extended pairing model [17] is given by

$$\hat{H} = \sum_{j=1}^{p} \epsilon_{j} n_{j} - G \sum_{i,j=1}^{p} b_{i}^{\dagger} b_{j} - G \sum_{\mu=2}^{\infty} \frac{1}{(\mu!)^{2}} \\ \times \sum_{i_{1} \neq i_{2} \neq \cdots \neq i_{2\mu}} b_{i_{1}}^{\dagger} b_{i_{2}}^{\dagger} \cdots b_{i_{\mu}}^{\dagger} b_{i_{\mu+1}} b_{i_{\mu+2}} \cdots b_{i_{2\mu}}, \qquad (2)$$

where G > 0 is the overall pairing strength. Besides the Nilsson mean field and the standard pairing interaction (1), the Hamiltonian (2) also includes many-pair hopping terms that allow nucleon pairs to simultaneously scatter (hop) between and among different Nilsson levels, which is thus simply exactly solvable. Due to the Pauli principle and the particle number conservation, the infinite sum in Eq. (2) naturally truncates, namely,  $\mu \leq \lfloor p/2 \rfloor$ , where  $\lfloor x \rfloor$  denotes the integer part of *x*. It is also clear that each term of the form  $b_i^{\dagger} \cdots b_j^{\dagger}$  that enters into the eigenstates of (2) should have different indices  $i \neq \cdots \neq j$ . Let  $\lfloor j_1, \ldots, j_m \rangle$  be the pairing vacuum state that satisfies

$$b_i|j_1,\ldots,j_m\rangle = 0 \tag{3}$$

for  $1 \le i \le p$ , where each of the *m* levels,  $j_1, j_2, \ldots, j_m$ , is occupied by a single nucleon. Following the algebraic Bethe ansatz used, one can write a *k*-pair eigenstate as

$$|k;\zeta;j_1,\ldots,j_m\rangle = \sum_{1\leqslant i_1<\cdots< i_k\leqslant p} C^{(\zeta)}_{i_1i_2\cdots i_k} b^{\dagger}_{i_1} b^{\dagger}_{i_2}\cdots b^{\dagger}_{i_k} |j_1,\ldots,j_m\rangle, \quad (4)$$

where  $C_{i_1i_2\cdots i_k}^{(\zeta)}$  are expansion coefficients that need to be determined. It is assumed that the levels  $j_1, j_2, \ldots, j_m$  should be excluded from the summation in Eq. (4). The expansion coefficient  $C_{i_1i_2\cdots i_k}^{(\zeta)}$  can be expressed very simply as

$$C_{i_{1}i_{2}\cdots i_{k}}^{(\zeta)} = \frac{1}{1 - \chi^{(\zeta)} \sum_{\mu=1}^{k} \epsilon_{i_{\mu}}},$$
(5)

where  $\chi^{(\zeta)}$  is a parameter that needs to be determined. In the seniority-zero cases, for example, directly applying the Hamiltonian (2) on the *k*-pair state (4) yields that for the mean-field part of (2)

$$\sum_{j} \epsilon_{j} n_{j} |k; \zeta; 0\rangle = \frac{2}{\chi^{(\zeta)}} \Biggl( |k; \zeta; 0\rangle - \sum_{1 \leq i_{1} < i_{2} < \dots < i_{k} \leq p} b_{i_{1}}^{\dagger} b_{i_{2}}^{\dagger} \cdots b_{i_{k}}^{\dagger} |0\rangle \Biggr), \tag{6}$$

and for the rearranged extended pairing part of (2)

$$\left(\sum_{i} b_{i}^{\dagger} b_{i} + \sum_{\mu=1}^{\infty} \frac{1}{(\mu!)^{2}} \sum_{i_{1} \neq i_{2} \neq \dots \neq i_{2\mu}} b_{i_{1}}^{\dagger} b_{i_{2}}^{\dagger} \dots b_{i_{\mu}}^{\dagger} b_{i_{\mu+1}} b_{i_{\mu+2}} \dots b_{i_{2\mu}}\right) |k; \zeta; 0\rangle$$

$$= \left(\sum_{1 \leq i_{1} < i_{2} < \dots < i_{k} \leq p} C_{i_{1}i_{2} \dots i_{k}}^{(\zeta)}\right) \sum_{1 \leq i_{1} < i_{2} < \dots < i_{k} \leq p} b_{i_{1}}^{\dagger} b_{i_{2}}^{\dagger} \dots b_{i_{k}}^{\dagger} |0\rangle + (k-1) |k; \zeta; 0\rangle.$$
(7)

By combining Eqs. (6) and (7), the k-pair eigenenergies of (2) are given by

$$E_k^{(\zeta)} = \frac{2}{\chi^{(\zeta)}} - G(k-1),$$
(8)

where  $\chi^{(\zeta)}$  should satisfy

$$\frac{2}{\chi^{(\zeta)}} + \sum_{1 \le i_1 < i_2 < \dots < i_k \le p} \frac{G}{\left(1 - \chi^{(\zeta)} \sum_{\mu=1}^k \epsilon_{i_\mu}\right)} = 0, \tag{9}$$

in which  $\chi^{(\zeta)}$  is the  $\zeta$ th solution of (9). Similar results for even-odd systems can also be derived by using this approach, except that the index *j* of the level occupied by the single nucleon should be excluded from the summation (4) and the single-particle energy  $\epsilon_j$  contributing to the eigenenergy from the first term of (2) should be included in Eq. (8). Extensions to many broken-pair cases are thus straightforward.

## III. BINDING ENERGIES AND EVEN-ODD MASS DIFFERENCES

As for any valence-shell model, the total energy of the ground state of a nuclear system is given by

$$E_B = E_B^{(\text{core})} + E_B(\nu) + E_B(\pi), \qquad (10)$$

where  $E_B^{(\text{core})}$  is the energy of the ground state of the core, taken to be <sup>132</sup>Sn in this study (reasonably approximated by a constant and given by the experimental binding energy of <sup>132</sup>Sn), and  $E_B(\nu)$  and  $E_B(\pi)$  are the lowest energies of the mean field and the residual pairing interaction for valence neutrons and protons, respectively, calculated either from Eq. (1) in the standard pairing model or from (2) in the extended pairing model, while the interaction between protons and neutrons is neglected in the present study. The neutron single-particle energies in Eqs. (1) and (2) are expressed as  $\epsilon_i(v) = \overline{\epsilon}_i(v) - \epsilon_0(v) - \epsilon(v)$ , and similarly for proton single-particle energies  $\epsilon_i(\pi)$ , where  $\overline{\epsilon}_i$  are the single-particle energies derived from the Nilsson model for open shell,  $\epsilon_0$  is the single-particle energy of the last Nilsson level filled by the core particles, which determines the zero-point energy in the Nilsson model for the valence particles, and  $\epsilon$  (>0) is the average binding energy per particle (neutron or proton), and is approximately taken to be a constant.

We consider a valence model space consisting of the sixth major shell with 22 Nilsson levels (orbits) for valence neutrons and 16 levels for valence protons. Hence, in our calculations, the total number of Nilsson levels is p = 22 for valence neutrons. Similarly, the total number of Nilsson levels for valence protons is p = 16. Finally, the odd-even mass difference is given by

$$P(A) = E_B(A+1) + E_B(A-1) - 2E_B(A),$$
(11)

where  $E_B(A)$  is the energy of the ground state of a nucleus with mass number A.

For each isotopic chain, by fitting to the experimental values of the binding energies, the odd-even mass differences, and the energies of the first pairing excitation states, the neutron  $G(\nu)$ and proton  $G(\pi)$  pairing interaction strengths and the average binding energy per particle  $\epsilon(\nu)$  and  $\epsilon(\pi)$  used in the extended pairing model are thus determined. The pairing interaction strengths  $G(\nu)$  and  $G(\pi)$  fitted for these isotopes are shown in Fig. 1. In addition, the best-fit parameter values for  $\epsilon$ are  $\epsilon(\nu) = 7.78$  MeV and  $\epsilon(\pi) = 5.82$  MeV for Er isotopes,  $\epsilon(\nu) = 8.04$  MeV and  $\epsilon(\pi) = 5.74$  MeV for Yb isotopes, and  $\epsilon(\nu) = 8.28$  MeV and  $\epsilon(\pi) = 5.00$  MeV for Hf isotopes.



FIG. 1. (Color online) Pairing interaction strengths G(v) and  $G(\pi)$  (in MeV) determined for the extended pairing model for <sup>152–164</sup>Er, <sup>154–166</sup>Yb, and <sup>156–168</sup>Hf.

To estimate the deviation between the predicted and experimental binding energies in a chain of isotopes, we use a root-mean-square deviation measure

$$\sigma = \left[ \sum_{\mu} \left( E_{B;\mu}^{\text{th}} - E_{B;\mu}^{\exp} \right)^2 \middle/ \mathcal{N} \right]^{1/2}, \qquad (12)$$

where  $E_{B;\mu}^{\text{th}}$  is the theoretical value of the ground-state energy,  $E_{B;\mu}^{\exp}$  is the corresponding experimental value [21],  $\mathcal{N}$  is the total number of nuclei in a chain fitted and the summation runs over all nuclei fitted in a chain. Namely, for the energy deviation, we obtain  $\sigma = 0.704$  MeV for the Er isotopes,  $\sigma = 0.819$  MeV for the Yb isotopes, and  $\sigma = 0.442$  MeV for the Hf isotopes.

The even-odd mass differences P(A) of the three chains of isotopes are calculated according to Eq. (11). These quantities are more sensitive to pairing correlations as compared to binding energies. As shown in Fig. 2, the even-odd mass differences of the three chains of isotopes are very close to the corresponding experimental data.

As shown in Fig. 1, the proton pairing interaction strength  $G(\pi)$  exhibits almost no change with mass number A because, for nuclei in an isotopic chain, the number of valence protons remains the same and also the proton-neutron interaction is neglected. In contrast, the neutron pairing interaction strength  $G(\nu)$  changes noticeably with increasing number of valence neutrons due to the fact that the pairing strength G in the extended pairing model is strongly dependent on the number of valence nucleon pairs [17,18]. According to [18], if only the first few eigenstates are considered, the pair structure of these



FIG. 2. (Color online) Theoretical and experimental even-odd mass differences (in MeV) for <sup>153–163</sup>Er, <sup>155–165</sup>Yb, and <sup>157–167</sup>Hf. Experimental values are denoted as "Exp.", and theoretical values calculated in the extended pairing model are denoted as "Th.".

states in the extended pairing model and the standard pairing model are similar, especially in the ground state. Moreover, when the number of pairs k or pairing interaction strength G is small, the difference between the two models is negligible. The parameter G in the extended pairing Hamiltonian (2) and the parameter  $G_{st}$  in the standard pairing Hamiltonian (1) satisfy the following relation [18]:

$$G = \frac{(p-k)!k!}{p!}(p-k+1)kG_{st}.$$
 (13)

The value of G in the extended pairing Hamiltonian (1) fitted for each nucleus shown in Fig. 1 and the corresponding value of  $G_{st}$  in the standard pairing Hamiltonian (2) obtained according to Eq. (13) is shown in Table I. Though the value of G shown in Fig. 1 seems small in the extended pairing model, the corresponding values of  $G_{st}$  in the standard pairing are reasonable as shown in Table I.

In addition, since the quantum number of the angular momentum projection along the third axis in the intrinsic frame is considered to be a conserved quantity, the excited states determined by the model can be regarded approximately as pairing excitation states with the same spin and parity as those of the ground state of a nucleus. The first pairing excitation states as calculated in the model are provided in Table II and are compared to experiment. As shown in Table II, there are some deviations between the theoretical results and the experimental data. One possible cause for such deviation is due to the fact that the proton-neutron quadrupole-quadrupole interaction is neglected in the model.

TABLE I. The pairing interaction strength  $G(v) [G(\pi)]$  (in MeV) in the extended pairing Hamiltonian (2) and the parameter  $G_{st}(v)$   $[G_{st}(\pi)]$  (in MeV) in the standard pairing Hamiltonian (1) for <sup>152–164</sup>Er, <sup>154–166</sup>Yb, and <sup>156–168</sup>Hf.

Nucleus	Α	G(v)	$G_{st}(v)$	$G(\pi)$	$G_{st}(\pi)$
<sup>152–164</sup> Er	152	0.3850	0.3850	0.0099	1.5730
	153	0.4600	0.4600	0.0097	1.5444
	154	0.0600	0.3300	0.0095	1.5145
	155	0.0730	0.4015	0.0093	1.4726
	156	0.0124	0.3185	0.0090	1.4348
	157	0.0122	0.3131	0.0088	1.3905
	158	0.0032	0.3119	0.0085	1.3467
	159	0.0037	0.3561	0.0082	1.3083
	160	0.0011	0.3217	0.0080	1.2679
	161	0.0014	0.4096	0.0077	1.2282
	162	0.0005	0.3330	0.0076	1.2150
	163	0.0003	0.2414	0.0072	1.1402
	164	0.0002	0.3502	0.0069	1.0963
<sup>154–166</sup> Yb	154	0.3900	0.3900	0.0149	1.7057
	155	0.4010	0.4010	0.0145	1.6603
	156	0.0590	0.3245	0.0141	1.6176
	157	0.0620	0.3410	0.0138	1.5747
	158	0.0127	0.3255	0.0133	1.5222
	159	0.0135	0.3465	0.0130	1.4821
	160	0.0031	0.3013	0.0128	1.4643
	161	0.0037	0.3561	0.0121	1.3831
	162	0.0010	0.3043	0.0117	1.3396
	163	0.0011	0.3219	0.0113	1.2944
	164	0.0004	0.3167	0.0109	1.2492
	165	0.0004	0.2926	0.0105	1.2035
	166	0.0002	0.3350	0.0101	1.1573
<sup>156–168</sup> Hf	156	0.1850	0.1850	0.0314	2.0755
	157	0.2700	0.2700	0.0304	2.0119
	158	0.0520	0.2860	0.0301	1.9923
	159	0.0614	0.3377	0.0288	1.9041
	160	0.0117	0.3000	0.0279	1.8481
	161	0.0127	0.3260	0.0271	1.7941
	162	0.0030	0.2888	0.0264	1.7479
	163	0.0034	0.3292	0.0256	1.6931
	164	0.0010	0.2938	0.0259	1.7132
	165	0.0011	0.3219	0.0247	1.6347
	166	0.0004	0.3007	0.0231	1.5268
	167	0.0004	0.2926	0.0223	1.4784
	168	0.0001	0.1523	0.0215	1.4196

#### **IV. MOMENT OF INERTIA**

The moments of inertia of the even-even nuclei in the three isotopic chains considered here and the even-odd differences of the moments of inertia of <sup>157–164</sup>Yb in the framework of the extended pairing model are also calculated. According to the Inglis cranking formula [22], the moment of inertia of a nucleus is calculated by

$$\Im = 2\hbar^2 \sum_{n} \frac{|\langle n | J_{x'} | 0 \rangle|^2}{E_n - E_0},$$
(14)

where  $J_{x'}$  is the total angular momentum along the intrinsic x' axis,  $|n\rangle$  is the *n*th excited state, and  $E_n$  is the corresponding

TABLE II. The first pairing excitation energy (in MeV) of  $^{156-164}$ Er,  $^{160-165}$ Yb, and  $^{166-168}$ Hf, where the values in the  $E^{\text{th}}$  and  $E^{\text{exp}}$  columns are the calculated pairing excitation energies and the corresponding experimental values taken from [23], respectively (energies not experimentally available are marked by "–").

Nucleus	Α	Spin and Parity	$E^{\exp}$	$E^{\mathrm{th}}$
<sup>156–164</sup> Er	156	$0_{2}^{+}$	0.930	1.360
	157	$\frac{3}{2}\frac{-}{2}$	0.110	0.444
	158	$0^{+}_{2}$	0.806	0.886
	159	$\frac{3}{22}$	_	0.231
	160	$0^{+}_{2}$	0.894	0.476
	161	$\frac{3}{2}$ -	0.725	0.375
	162	$0^+_2$	1.087	1.264
	163	$\frac{5}{22}$	0.164	0.359
	164	$0^+_2$	1.246	1.870
<sup>160–165</sup> Yb	160	$0^+_2$	1.086	0.791
	161	$\frac{3}{2}\frac{-}{2}$	0.211	0.386
	162	$0^{+}_{2}$	0.606	0.487
	163	$\frac{3}{22}$	0.871	0.559
	164	$0^{+}_{2}$	0.976	0.325
	165	$\frac{5}{2}\frac{-}{2}$	0.174	0.190
<sup>166–168</sup> Hf	166	$0_2^+$	0.695	0.387
	167	$\frac{5}{2}\frac{-}{2}$	-	0.106
	168	$0_{2}^{+}$	0.942	1.298

excitation energy. In principle, the summation in Eq. (14) should run over all excited states. As a good approximation, only the pairing case and one broken pair case are taken into account in our calculations. This approximation is justified since excited states with two or more broken pairs lie much higher in energy above the ground state and their contribution to the moment of inertia (14) is negligible [24]. The matrix elements of  $J_{x'}$  used in Eq. (14) for both even-even and odd-*A* nuclei are provided in Appendix A.

In this paper, the moments of inertia of the even-even nuclei considered are all calculated. However, only the moments of inertia of odd Yb nuclei are calculated because either the spin or the first excited level energy in the ground-state band in odd Er or odd Hf nuclei is not available experimentally. The difference of the spins of adjacent levels in the ground-state band with bandhead spin  $\Omega$  satisfies  $\Delta I = 1$  in <sup>161</sup>Yb, of which the experimental value of the moment of inertia is obtained according to Eq. (B3) shown in Appendix B, while the difference of the spins of adjacent levels in the ground-state band with bandhead spin  $\Omega$  satisfies  $\Delta I = 2$  in <sup>163,165</sup>Yb, of which the experimental values of the moments of inertia are obtained according to Eq. (B4) provided in Appendix B. The level energies of these isotopes are all taken form [25]. For <sup>157</sup>Yb and <sup>159</sup>Yb, the total spin I of the first excited state in the groundstate band is also not observed experimentally. Hence, the experimental moments of inertia of <sup>157</sup>Yb and <sup>159</sup>Yb are absent.

The calculated moments of inertia and the corresponding experimental data for the even-even nuclei in the three isotopic



FIG. 3. (Color online) Theoretical and experimentally deduced values of the moment of inertia in  $\hbar^2 \text{MeV}^{-1}$  for even-even <sup>154–162</sup>Er, <sup>156–164</sup>Yb, and <sup>158–166</sup>Hf, where "Ext." denotes theoretical results obtained in the extended pairing model, "Nil." denotes theoretical results obtained in the Nilsson mean field without pairing interaction, and the values denoted by "Exp." are extracted from the experimental spectra of these nuclei [25] according to (B2).

chains are shown in Fig. 3. It shows that the results obtained from the Nilsson mean-field plus extended-pairing model are in excellent agreement with the corresponding experimental data. For comparison, the moments of inertia obtained by the Inglis formula from the Nilsson mean field without pairing interaction are also provided, though the difference in calculated moments of inertia with and without pairing interaction has been well known [26,27].

Similar to the definition of the odd-even mass difference, the relative odd-even difference of the moments of inertia may be defined as [27]

$$P_{\mathfrak{Z}} = \frac{\delta\mathfrak{Z}}{\mathfrak{Z}} \bigg|_{\mathrm{av}} = \frac{\mathfrak{Z}(A) - \frac{1}{2}[\mathfrak{Z}(A+1) + \mathfrak{Z}(A-1)]}{\frac{1}{2}[\mathfrak{Z}(A+1) + \mathfrak{Z}(A-1)]}, \quad (15)$$

where A is the mass number and  $\frac{1}{2}[\Im(A+1) + \Im(A-1)]$  is the average of the ground-state band moments of inertia of the neighboring nuclei.

The theoretical and experimental values of the moment of inertia  $\Im$  for both even-even and odd-*A* Yb nuclei are shown in Fig. 4(a). The relative odd-even differences of the moments of inertia  $P_{\Im}$  for Yb are shown in Fig. 4(b). Clearly, the theoretical values of the moment of inertia are in a good agreement with the corresponding experimentally deduced values for even-even nuclei, while there are small deviations between the theoretical and experimental moments of inertia for odd-*A* nuclei.



FIG. 4. (Color online) (a) Theoretical and experimentally deduced moments of inertia in  $\hbar^2 \text{MeV}^{-1}$  for <sup>156–165</sup>Yb, where "Ext." denotes results obtained in the extended pairing model, and "Exp." denotes the corresponding values extracted from the experimental spectra of these nuclei [25] according to (B2) for even-even nuclei and (B3) or (B4) for odd-*A* nuclei. (b) Relative evenodd differences of the moments of inertia of <sup>157–164</sup>Yb, calculated by (15), where experimental data is denoted by "Exp." and theoretical values in the extended pairing model are denoted as "Ext.".

# V. GROUND-STATE OCCUPATION PROBABILITIES OF VALENCE NUCLEON PAIRS WITH VARIOUS ANGULAR MOMENTUM QUANTUM NUMBERS

In this section, we calculate the ground-state occupation probabilities of valence nucleon pairs with various angular momentum quantum numbers for even-even nuclei in the extended pairing model. Our aim is to identify angular momentum values of valence pairs that are important in the ground state of these nuclei.

For the *i*th Nilsson level, the pair creation operators  $b_i^{\dagger}$  can be expressed in terms of the single-particle creation operators of the spherical harmonic oscillator shell model,

$$b_{i}^{\dagger} = \sum_{j_{i}j_{i}^{\prime}} W_{j_{i}}^{i} W_{j_{i}^{\prime}}^{i} (-)^{j_{i}^{\prime} - \Omega_{i}} c_{j_{i}\Omega_{i}}^{\dagger} c_{j_{i}^{\prime}\overline{\Omega}_{i}}^{\dagger}, \qquad (16)$$

where  $c_{j_i\Omega_i}^{\dagger}$  are the single-particle creation operators with definite angular momentum quantum number  $j_i$ ,  $\Omega_i$  is the projection of  $j_i$  onto the third axis of the intrinsic frame, and  $W_{j_i}^i$ , as shown in Eq. (A9), are normalized expansion coefficients of the *i*th Nilsson state expanded in terms of a set of spherical shell model states. In addition,

$$c_{j_i\Omega_i}^{\dagger}c_{j_i^{\prime}\overline{\Omega}_i}^{\dagger} = \sum_{J_i} \langle j_i\Omega_i j_i^{\prime}\overline{\Omega}_i | J_i 0 \rangle B_{j_i j_i^{\prime} J_i 0}^{\dagger}, \qquad (17)$$

where  $\langle j_i \Omega_i j'_i \overline{\Omega}_i | J_i 0 \rangle$  is a Clebsch-Gordan coefficient, and  $B^{\dagger}_{j_i j'_i J_i 0}$  is the pairing operator with total angular momentum



FIG. 5. (Color online) Ground state occupation probabilities of valence nucleon pairs with angular momentum quantum number J in <sup>156–162</sup>Yb calculated in the Nilsson mean-field plus extended-pairing model.

quantum number  $J_i$ . Thus, we also have

$$B_{j_ij_i'J_i0}^{\dagger} = \sum_{j_ij_i'} \langle j_i \Omega_i j_i' \overline{\Omega} | J_i 0 \rangle c_{j_i \Omega_i}^{\dagger} c_{j_i' \overline{\Omega}_i}^{\dagger}.$$
(18)

By substituting (17) into (16), Eq. (16) becomes

$$b_{i}^{\dagger} = \sum_{j_{i}j_{i}'} W_{j_{i}}^{i} W_{j_{i}'}^{i} (-)^{j_{i}' - \Omega_{i}} \sum_{J_{i}} \langle j_{i} \Omega_{i} j_{i}' \overline{\Omega}_{i} | J_{i} 0 \rangle B_{j_{i}j_{i}'J_{i}0}^{\dagger}.$$
 (19)

By substituting (19) into (4), the  $k^{\rho}$ -pair eigenstates of the model can be expressed as

$$|k^{\rho};\zeta;0\rangle = \sum_{1\leqslant i_{1}<\cdots< i_{k}\leqslant p} C^{(\zeta)}_{i_{1}i_{2}\cdots i_{k}} \prod_{i=1}^{k^{\rho}} \left(\sum_{j_{i}j'_{i}} W^{i}_{j_{i}}W^{i}_{j'_{i}}(-)^{j'_{i}-\Omega_{i}}\right)$$
$$\times \sum_{J_{i}} \langle j_{i}\Omega_{i}j'_{i}\overline{\Omega_{i}}|J_{i}0\rangle B^{\dagger}_{j_{i}j'_{i}J_{i}0}(\rho) \left|0\rangle, \qquad (20)$$

where  $\rho = \pi$  for protons or  $\rho = \nu$  for neutrons.

The number of like-nucleon pairs with angular momentum *J* in the ground state can then be calculated by

$$n_{J}^{\rho} = \langle k^{\rho}; \zeta = 1; 0 | \sum_{jj'} B^{\dagger}_{jj'J0}(\rho) \frac{\partial}{\partial B^{\dagger}_{jj'J0}(\rho)} | k^{\rho}; \zeta = 1; 0 \rangle,$$
(21)

which counts the number of like-nucleon pairs with angular momentum J in the ground state. Since both the proton and neutron sectors are considered in this work, the ground state occupation probability of valence nucleon pairs with angular momentum J in the model can be expressed as

$$\eta_J = \frac{n_J^\pi + n_J^\nu}{k},\tag{22}$$

where the total number of pairs is  $k = k^{\pi} + k^{\nu}$ .

Figure 5 displays the calculated results for the ground state occupation probabilities of valence nucleon pairs with angular momentum J = 0 to J = 12 for  $^{156-162}$ Yb. It is obvious that the pair occupation probability decreases with increasing J and is much higher for even-J pairs as compared to odd-J pairs. Moreover, among the occupation probabilities of even-J pairs, those with J = 0, 2, and 4 are the three highest ones. However, the occupation probabilities of J = 6 and J = 8 pairs, even those of J = 10 and J = 12 pairs, are non-negligible. Fig. 5 also shows that the above conclusions are independent of the number of valence nucleon pairs k and, therefore, hold for any k cases.

Anyway, the results shown in Fig. 5 reveal that, in the framework of the Nilsson mean-field plus extended-pairing model, the *S*, *D*, and *G* valence nucleon pairs dominate in the ground state of these nuclei. The total occupation probability of *S*, *D*, and *G* valence nucleon pairs is higher than 60%, while other even-*J* pairs also contribute to the ground state noticeably. In addition, our analysis shows that the *G*-pair contribution to the ground state of these nuclei is also significant. Hence, the IBM with *s*, *d*, and *g* bosons seems to provide a reasonable simplified description of the collective motion of these deformed nuclei [28].

### **VI. CONCLUSION**

In summary, the Nilsson mean-field plus extended-pairing model for well-deformed nuclei is applied to describe rare earth nuclei. Binding energies, energies of the first pairing excitation states, even-odd mass differences, and moments of inertia of <sup>152–164</sup>Er, <sup>154–166</sup>Yb, and <sup>156–168</sup>Hf are calculated systematically in the model with both proton-proton and neutron-neutron pairing interactions. We find that, for these three chains of isotopes, the outcomes of the model, with only four adjustable parameters (proton and neutron pairing strengths and the average binding energy per nucleon), reproduce rather well the corresponding experimental values of binding energies, even-odd mass differences, and moments of inertia. The analysis shows that pairing interaction is crucial in elucidating spectral properties of these nuclei. However, observed small deviations in the energy of the first pairing excitation states predicted in the model from the corresponding experimental results may result from the fact that the proton-neutron quadrupole-quadrupole interaction is neglected.

Ground-state occupation probabilities of valence nucleon pairs with angular momentum quantum number J in  $^{156-162}$ Yb are also calculated. The model outcome suggests that the even-J pair occupation probabilities are much higher than the odd-J ones. Most importantly, we find that S, D, and Gpairs dominate in the ground state of these nuclei. Though the ground-state occupation probabilities of valence nucleon pairs with angular momentum quantum number J in <sup>156–162</sup>Yb are calculated by using the Nilsson plus extended-pairing model, the results seem independent of the specific pairing model used. For example, one can also calculate these occupation probabilities by using the Nilsson mean field and the standard pairing model, which should yield results similar to those shown in this paper. As shown in Ref. [16], in which the Nilsson mean field plus the standard pairing model was used to analyze the angular momentum decomposition of only one valence neutron pair, the result of the case studied and the conclusions made are quite similar to the ones shown in this work. Hence, the IBM with s, d, and g bosons seems to provide a reasonable simplified description of the collective motion of these deformed nuclei. Our analysis thus provides a fermionic shell-model reasoning for IBM studies.

In addition, by comparing our model calculations with experimental data, we provide a reasonable range of pairing interaction strength G, with which the quantum phase transition and related critical phenomena induced by the competition of the deformed mean-field and the pairing interaction can further be analyzed as suggested in Ref. [29]. Moreover, since the total angular momentum is not conserved in the model and proton-neutron quadrupole-quadrupole interaction is neglected in this work, it should be interesting to explore more realistic situations to take these issues into account. For example, the results of this work may be used to investigate excited states in the model by using the angular momentum projection technique, which will be a part of our future work.

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# APPENDIX A: THE MATRIX ELEMENTS OF $J_{x'}$

In the Nilsson basis,  $J_{x'}$  can be expressed as

$$J_{x'} = \sum_{j_{\beta}\Omega_{\beta}j_{\beta'}\Omega_{\beta'}} \langle j_{\beta}\Omega_{\beta} | J_{x'} | j_{\beta'}\Omega_{\beta'} \rangle a^{\dagger}_{j_{\beta}\Omega_{\beta}} a_{j_{\beta'}\Omega_{\beta'}}.$$
(A1)

For even-even case, when the two valence nucleons are in the Nilsson states  $(j_{\rho}\Omega_{\rho}, j_{\gamma}\Omega_{\gamma})$ , the matrix element of  $J_{x'}$  can be written as

$$\langle k-1; \zeta'; j_{\rho} \Omega_{\rho}, j_{\gamma} \Omega_{\gamma} | J_{x'} | k, \zeta = 1; 0 \rangle$$

$$= \sum_{p=1}^{k} \sum_{i_{1} < \dots < i_{p-1} < i_{p+1} < \dots < i_{k}} C_{i_{1}i_{2} \cdots i_{p-1}i_{p+1} \cdots i_{k}}^{(\zeta')}$$

$$\times \left( C_{i_{1}i_{2} \dots i_{p-1}j_{\rho}i_{p+1} \dots i_{k}}^{(\zeta)} \langle j_{\gamma} \Omega_{\gamma} | J_{x'} | j_{\rho} \bar{\Omega}_{\rho} \rangle \delta_{i_{p}j_{\rho}} - C_{i_{1}i_{2} \dots i_{p-1}j_{\gamma}i_{p+1} \dots i_{k}}^{(\zeta)} \langle j_{\rho} \Omega_{\rho} | J_{x'} | j_{\gamma} \bar{\Omega}_{\gamma} \rangle \delta_{i_{p}j_{\gamma}} \right).$$
(A2)

When the two valence nucleons are in the Nilsson states  $(j_{\rho}\Omega_{\rho}, j_{\gamma}\bar{\Omega}_{\gamma})$ , the matrix element of  $J_{x'}$  can be written as

$$\langle k-1; \zeta'; j_{\rho} \Omega_{\rho}, j_{\gamma} \Omega_{\gamma} | J_{x'} | k, \zeta = 1; 0 \rangle$$

$$= \sum_{p=1}^{k} \sum_{i_{1} < \cdots < i_{p-1} < i_{p+1} < \cdots < i_{k}} C_{i_{1}i_{2} \cdots i_{p-1}i_{p+1} \cdots i_{k}}^{(\zeta')}$$

$$\times \left( C_{i_{1}i_{2} \cdots i_{p-1}j_{\rho}i_{p+1} \cdots i_{k}}^{(\zeta)} \langle j_{\gamma} \bar{\Omega}_{\gamma} | J_{x'} | j_{\rho} \bar{\Omega}_{\rho} \rangle \delta_{i_{p}j_{\rho}} \right.$$

$$\left. + C_{i_{1}i_{2} \cdots i_{p-1}j_{\gamma}i_{p+1} \cdots i_{k}}^{(\zeta)} \langle j_{\rho} \Omega_{\rho} | J_{x'} | j_{\gamma} \Omega_{\gamma} \rangle \delta_{i_{p}j_{\gamma}} \right).$$
(A3)

When the two valence nucleons are in the Nilsson states  $(j_{\rho}\bar{\Omega}_{\rho}, j_{\gamma}\bar{\Omega}_{\gamma})$ , the matrix element of  $J_{x'}$  can be written as

$$\begin{split} \langle k - 1; \zeta'; j_{\rho} \bar{\Omega}_{\rho}, j_{\gamma} \bar{\Omega}_{\gamma} | J_{x'} | k, \zeta &= 1; 0 \rangle \\ &= \sum_{p=1}^{k} \sum_{i_{1} < \cdots < i_{p-1} < i_{p+1} < \cdots < i_{k}} C^{(\zeta')}_{i_{1}i_{2} \cdots i_{p-1}i_{p+1} \cdots i_{k}} \\ &\times \left( -C^{(\zeta)}_{i_{1}i_{2} \dots i_{p-1}j_{\rho}i_{p+1} \dots i_{k}} \langle j_{\gamma} \bar{\Omega}_{\gamma} | J_{x'} | j_{\rho} \Omega_{\rho} \rangle \delta_{i_{p}j_{\rho}} \right. \\ &+ C^{(\zeta)}_{i_{1}i_{2} \dots i_{p-1}j_{\gamma}i_{p+1} \dots i_{k}} \langle j_{\rho} \bar{\Omega}_{\rho} | J_{x'} | j_{\gamma} \Omega_{\gamma} \rangle \delta_{i_{\rho}j_{\gamma}} \Big). \end{split}$$
(A4)

For the odd-A case, when the three valence nucleons are in the Nilsson states  $(j_{\rho}\Omega_{\rho}, j_{\gamma}\Omega_{\gamma}, j_{\mu}\Omega_{\mu})$ , the matrix element of  $J_{x'}$  can be written as

$$\begin{split} \langle k - 1, \zeta', j_{\rho} \Omega_{\rho}, j_{\gamma} \Omega_{\gamma}, j_{\mu} \Omega_{\mu} | J_{x'} | k, \zeta &= 1; j'_{\mu} \Omega'_{\mu} \rangle \\ &= \sum_{p=1}^{k} \sum_{i_{1} < i_{2} < \cdots < i_{p-1} < i_{p+1} < \cdots < i_{k}} C_{i_{1}i_{2} \dots i_{p-1}i_{p+1} \cdots i_{k}}^{(\zeta')} \\ &\times \left[ C_{i_{1}i_{2} \dots i_{p-1}j_{\gamma}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\mu} \Omega_{\mu} | J_{x'} | j_{\gamma} \bar{\Omega}_{\gamma} \rangle \delta_{j_{\rho}j'_{\mu}} \right. \\ &- \langle j_{\rho} \Omega_{\rho} | J_{x'} | j_{\gamma} \bar{\Omega}_{\gamma} \rangle \delta_{j_{\mu}j'_{\mu}} \right) \delta_{i_{p}j_{\gamma}} \\ &+ C_{i_{1}i_{2} \dots i_{p-1}j_{\rho}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\gamma} \Omega_{\gamma} | J_{x'} | j_{\rho} \bar{\Omega}_{\rho} \rangle \delta_{j_{\mu}j'_{\mu}} \right. \\ &- \langle j_{\mu} \Omega_{\mu} | J_{x'} | j_{\rho} \bar{\Omega}_{\rho} \rangle \delta_{j_{\gamma}j'_{\mu}} \right) \delta_{i_{p}j_{\rho}} \\ &+ C_{i_{1}i_{2} \dots i_{p-1}j_{\mu}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\rho} \Omega_{\rho} | J_{x'} | j_{\mu} \bar{\Omega}_{\mu} \rangle \delta_{j_{\gamma}j'_{\mu}} \right. \\ &- \langle j_{\gamma} \Omega_{\gamma} | J_{x'} | j_{\mu} \bar{\Omega}_{\mu} \rangle \delta_{j_{\rho}j'_{\mu}} \right) \delta_{i_{p}j_{\mu}} \bigg]. \end{split}$$

When the three valence nucleons are in the Nilsson states  $(j_{\rho}\Omega_{\rho}, j_{\gamma}\bar{\Omega}_{\gamma}, j_{\mu}\Omega_{\mu})$ , the matrix element of  $J_{x'}$  can be written as

$$\begin{split} \langle k - 1, \zeta', j_{\rho} \Omega_{\rho}, j_{\gamma} \bar{\Omega}_{\gamma}, j_{\mu} \Omega_{\mu} | J_{x'} | k, \zeta &= 1; j'_{\mu} \Omega'_{\mu} \rangle \\ &= \sum_{p=1}^{k} \sum_{i_{1} < i_{2} < \cdots < i_{p-1} < i_{p+1} < \cdots < i_{k}} C_{i_{1}i_{2} \ldots i_{p-1}i_{p+1} \cdots i_{k}}^{(\zeta')} \\ &\times \Big[ -C_{i_{1}i_{2} \ldots i_{p-1}j_{\gamma}i_{p+1} \cdots i_{k}}^{(\zeta)} (\langle j_{\mu} \Omega_{\mu} | J_{x'} | j_{\gamma} \Omega_{\gamma} \rangle \delta_{j_{\rho}j'_{\mu}} \\ &- \langle j_{\rho} \Omega_{\rho} | J_{x'} | j_{\gamma} \Omega_{\gamma} \rangle \delta_{j_{\mu}j'_{\mu}} )\delta_{i_{p}j_{\gamma}} \\ &+ C_{i_{1}i_{2} \ldots i_{p-1}j_{\rho}i_{p+1} \cdots i_{k}}^{(\zeta)} (\langle j_{\gamma} \Omega_{\gamma} | J_{x'} | j_{\rho} \bar{\Omega}_{\rho} \rangle \delta_{j_{\mu}j'_{\mu}} \\ &- \langle j_{\mu} \Omega_{\mu} | J_{x'} | j_{\rho} \bar{\Omega}_{\rho} \rangle \delta_{j_{\gamma}j'_{\mu}} )\delta_{i_{p}j_{\rho}} \\ &+ C_{i_{1}i_{2} \ldots i_{p-1}j_{\mu}i_{p+1} \cdots i_{k}}^{(\zeta)} (\langle j_{\rho} \Omega_{\rho} | J_{x'} | j_{\mu} \bar{\Omega}_{\mu} \rangle \delta_{j_{\gamma}j'_{\mu}} \\ &- \langle j_{\gamma} \Omega_{\gamma} | J_{x'} | j_{\mu} \bar{\Omega}_{\mu} \rangle \delta_{j_{\rho}j'_{\mu}} \Big]. \end{split}$$

When the three valence nucleons are in the Nilsson states  $(j_{\rho}\bar{\Omega}_{\rho}, j_{\gamma}\bar{\Omega}_{\gamma}, j_{\mu}\Omega_{\mu})$ , the matrix element of  $J_{x'}$  can be written as

$$\langle k - 1, \zeta', j_{\rho} \bar{\Omega}_{\rho}, j_{\gamma} \bar{\Omega}_{\gamma}, j_{\mu} \Omega_{\mu} | J_{x'} | k, \zeta = 1; j'_{\mu} \Omega'_{\mu} \rangle$$

$$= \sum_{p=1}^{k} \sum_{i_{1} < i_{2} < \cdots < i_{p-1} < i_{p+1} < \cdots < i_{k}} C_{i_{1}i_{2} \cdots i_{p-1}i_{p+1} \cdots i_{k}}^{(\zeta')} \\ \times \left[ -C_{i_{1}i_{2} \cdots i_{p-1}j_{\gamma}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\mu} \Omega_{\mu} | J_{x'} | j_{\gamma} \Omega_{\gamma} \rangle \delta_{j_{\rho}j'_{\mu}} \right. \right. \\ \left. - \langle j_{\rho} \bar{\Omega}_{\rho} | J_{x'} | j_{\gamma} \Omega_{\gamma} \rangle \delta_{j_{\mu}j'_{\mu}} \right) \delta_{i_{p}j_{\gamma}} \\ \left. - C_{i_{1}i_{2} \cdots i_{p-1}j_{\rho}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\gamma} \bar{\Omega}_{\gamma} | J_{x'} | j_{\rho} \Omega_{\rho} \rangle \delta_{j_{\mu}j'_{\mu}} \right. \\ \left. - \langle j_{\mu} \Omega_{\mu} | J_{x'} | j_{\rho} \Omega_{\rho} \rangle \delta_{j_{\gamma}j'_{\mu}} \right) \delta_{i_{p}j_{\rho}} \\ \left. + C_{i_{1}i_{2} \cdots i_{p-1}j_{\mu}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\rho} \bar{\Omega}_{\rho} | J_{x'} | j_{\mu} \bar{\Omega}_{\mu} \rangle \delta_{j_{\gamma}j'_{\mu}} \right. \\ \left. - \langle j_{\gamma} \bar{\Omega}_{\gamma} | J_{x'} | j_{\mu} \bar{\Omega}_{\mu} \rangle \delta_{j_{\rho}j'_{\mu}} \right) \delta_{i_{p}j_{\mu}} \right].$$

When the three valence nucleons are in the Nilsson states  $(j_{\rho}\bar{\Omega}_{\rho}, j_{\gamma}\bar{\Omega}_{\gamma}, j_{\mu}\bar{\Omega}_{\mu})$ , the matrix element of  $J_{x'}$  can be written as

$$\langle k - 1, \zeta', j_{\rho} \overline{\Omega}_{\rho}, j_{\gamma} \overline{\Omega}_{\gamma}, j_{\mu} \overline{\Omega}_{\mu} | J_{x'} | k, \zeta = 1; j'_{\mu} \Omega'_{\mu} \rangle$$

$$= \sum_{p=1}^{k} \sum_{i_{1} < i_{2} < \cdots < i_{p-1} < i_{p+1} < \cdots < i_{k}} C_{i_{1}i_{2} \dots i_{p-1}i_{p+1} \cdots i_{k}}^{(\zeta')} \\ \times \left[ -C_{i_{1}i_{2} \dots i_{p-1}j_{\gamma}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\mu} \overline{\Omega}_{\mu} | J_{x'} | j_{\gamma} \Omega_{\gamma} \rangle \delta_{j_{\rho}j'_{\mu}} \right. \\ \left. - \langle j_{\rho} \overline{\Omega}_{\rho} | J_{x'} | j_{\gamma} \Omega_{\gamma} \rangle \delta_{j_{\mu}j'_{\mu}} \right) \delta_{i_{p}j_{\gamma}} \\ \left. - C_{i_{1}i_{2} \dots i_{p-1}j_{\rho}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\gamma} \overline{\Omega}_{\gamma} | J_{x'} | j_{\rho} \Omega_{\rho} \rangle \delta_{j_{\mu}j'_{\mu}} \right. \\ \left. - \langle j_{\mu} \overline{\Omega}_{\mu} | J_{x'} | j_{\rho} \Omega_{\rho} \rangle \delta_{j_{\gamma}j'_{\mu}} \right) \delta_{i_{p}j_{\rho}} \\ \left. - C_{i_{1}i_{2} \dots i_{p-1}j_{\mu}i_{p+1} \cdots i_{k}}^{(\zeta)} \left( \langle j_{\rho} \overline{\Omega}_{\rho} | J_{x'} | j_{\mu} \Omega_{\mu} \rangle \delta_{j_{\gamma}j'_{\mu}} \right. \\ \left. - \langle j_{\gamma} \overline{\Omega}_{\gamma} | J_{x'} | j_{\mu} \Omega_{\mu} \rangle \delta_{j_{\rho}j'_{\mu}} \right] \right\}$$

$$(A8)$$

044303-8

It should be noted that the Nilsson orbits occupied by the unpaired particles,  $j_{\rho}$ ,  $j_{\gamma}$ , and  $j_{\mu}$  should be excluded in the summation in Eqs. (A2)–(A8). In Eq. (14), only excited states up to one broken pair are considered. By substituting these matrix elements into (14), one obtains a good estimate of the moment of inertia of a nucleus. This is a reasonable approximation as long as the quantum number of the total angular momentum is small. Therefore, (14) can be also used to calculate the moment of inertia of a nucleus for the first excited state in the ground-state band. In order to obtain the matrix elements of  $J_{x'}$ , the *i*th Nilsson single-particle states are expanded in terms of single-particle states  $|Nj\Omega_i\rangle$  of the spherical harmonic oscillator shell model with

$$|i; \Omega_i\rangle = \sum_j W_j^i |Nj\Omega_i\rangle,$$
  
$$|i; \bar{\Omega}_i\rangle = \sum_j W_j^i (-)^{j-\Omega_i} |Nj - \Omega_i\rangle,$$
 (A9)

where N is the principal quantum number, which is fixed according to the major shell used in our calculations, j is the total angular momentum quantum number, i labels the *i*th Nilsson level, and  $W_j^i$  are expansion coefficients. The total angular momentum j is obtained by coupling the orbital angular moment l with the spin s = 1/2 of a valence nucleon. For example, since  $J_{x'}$  only changes  $\Omega_i$ ,

$$\langle Nj'\Omega_{i'}|J_{x'}|Nj\Omega_i\rangle = \langle j\Omega_{i'} \pm 1|J_{x'}|j\Omega_i\rangle\delta_{jj'}\delta_{\Omega_{i'}\Omega_i\pm 1}, \quad (A10)$$

where  $\langle j\Omega_i \pm 1 | J_{x'} | j\Omega_i \rangle = \frac{\hbar}{2} \sqrt{(j \pm \Omega_i + 1)(j \mp \Omega_i)}$ , the matrix elements of  $J_{x'}$  in the Nilsson basis can be expressed as

$$\langle i'; \Omega_{i'} | J_{x'} | i; \Omega_i \rangle = \sum_j W_j^{i'} W_j^i \frac{\hbar}{2} \sqrt{(j \pm \Omega_i + 1)(j \mp \Omega_i)} \delta_{\Omega_{i'}\Omega_i \pm 1}, \quad (A11)$$

which is used in Eqs. (A2)–(A8).

# APPENDIX B: EXPERIMENTAL VALUE OF THE MOMENT OF INERTIA

The experimental value of the moment of inertia of a deformed nucleus is extracted from the rotational spectrum, which is assumed to be described by the particle-rotor model with eigenenergy

$$E(I) = E_{\Omega} + \frac{\hbar^2}{2\Im} [I(I+1) + \delta_{\Omega,1/2} a(-1)^{I+1/2} (I+1/2)]$$
(B1)

for given total spin I and the quantum number of its third component in the intrinsic frame  $\Omega$ , and a is the decoupling factor. Within a rotational band,  $E_{\Omega}$  is a constant. Moreover, since the Inglis formula is derived perturbatively, it only applies to excited states with small angular momentum quantum number. Therefore, according to (B1), for even-even nuclei, the experimental value of the moment of inertia is then obtained with

$$\frac{2\Im_{\text{Exp.}}}{\hbar^2} = \frac{6}{E(2^+_1) - E(0^+_g)} \equiv \frac{6}{E(2^+_1)},$$
 (B2)

where  $E(2_1^+)$  is the energy of the first  $2^+$  excited state taken from the experimental spectrum. Similarly, for odd-A nuclei, if an  $\Omega \neq 1/2$  band is considered, which is always the case for the ground-state band studied in this paper, the decoupling term in Eq. (B1) is zero. The experimental value of the moment of inertia can then be obtained either as

$$\frac{2\Im_{\text{Exp.}}}{\hbar^2} = \frac{2(\Omega+1)}{E(\Omega+1) - E(\Omega)} \equiv \frac{2(\Omega+1)}{E(\Omega+1)},$$
 (B3)

if the difference of the spins of adjacent levels in the groundstate band with bandhead spin  $\Omega$  satisfies  $\Delta I = 1$ , or as

$$\frac{2\Im_{\text{Exp.}}}{\hbar^2} = \frac{2(2\Omega+3)}{E(\Omega+2) - E(\Omega)} \equiv \frac{2(2\Omega+3)}{E(\Omega+2)}, \quad (B4)$$

if the difference of the spins of adjacent levels in the groundstate band with bandhead spin  $\Omega$  satisfies  $\Delta I = 2$ , where  $E(\Omega + 1)$  or  $E(\Omega + 2)$  is the experimental energy of the first excited state in the ground-state band.

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