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Ground-state Properties of Er, Yb and Hf Isotopes

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Abstract: 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, 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. In comparison with the corresponding experimental data, it is shown that for these rare-earth nuclei, pairing interaction is crucial in elucidating the properties of the ground state. With model parameters determined by fitting the energies of these states, ground-state occupation probabilities of valence nucleon pairs with angular momentum $J=0,1,\cdots,12$ for even-even $^{156-162}$Yb are calculated. It is inferred that the occupation probabilities of valence nucleon pairs with even angular momenta are much higher than those 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.

Key words: ground state occupation probability; pairing interaction strength; Nilsson mean-field plus extended-pairing model

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1 Introduction

Nuclear pairing correlation, similar to the pairing correlation in the Bardeen-Cooper-Schrieffer (BCS) theory of superconductors, is a key ingredient from the residual interactions of the nuclear shell model in elucidating properties of the ground states and low-energy spectra of nuclei, such as binding energies, odd-even effects, single-particle occupancies, excitation spectra, electromagnetic transition rates, beta-decay probabilities, and so on[1–5]. However, both the BCS theory and the more refined Hartree-Fock-Bogolyubov (HFB) methods suffer from serious drawbacks in nuclear systems due to the violation of particle-number conservation. A remedy in terms of particle number projection complicates the algorithms considerably, often without yielding a better description of higher-lying excited states that is a natural part of the spectrum of the pairing Hamiltonian[6–8]. Also, due to the limitation of computing power for the calculations in heavy nuclei, truncation schemes have to be employed. The Projected Shell Model (PSM) provides a way to overcome this difficulty[9]. 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 fermion pair system[10]. Nevertheless, tremendous success of the interacting boson model (IBM)[11] suggests that S and D pairs play a dominant role in low-lying part of the spectroscopy[12, 13]. It is indicated that, by using the exact solutions of the pairing model (Richardson-Gaudin method), the angular momentum distribution of the Richardson pairs in different kind of nuclei, going from spherical to deformed ones, can be used to clarify the microscopic foundation of IBM[14].

More recently, the Nilsson mean-field plus extended-pairing model[15–17] for deformed nuclei is applied to describe the ground-state properties of some rare-earth nuclei. Binding energies, even-odd mass differences, energies of the first pairing excitation states, 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[18]. It is indicated 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

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the corresponding experimental values of binding energies, even-odd mass differences, and moments of inertia rather well. Ground-state occupation probabilities of valence nucleon pairs with angular momentum quantum number J in $^{156-162}$Yb are also calculated in the Nilsson mean-field plus the extended-pairing model[18]. The model results show that the even-J pair occupation probabilities are much higher than the odd-J ones. Most importantly, we find that S, D, and G pairs dominate in the ground state of these nuclei. Hence, the IBM with s-, d-, and g-bosons seems a reasonable simplified description of the collective motion of these deformed nuclei. Our analysis thus provides a fermionic shell-model reasoning for the IBM description.

2 The extended pairing model

The Hamiltonian of the extended pairing model[15] is given by

$$\hat{H}=\sum_{i=1}^{p}\epsilon_i n_i - G\sum_{i,i'=1}^{p} b_i^{\dagger} b_{i'} - G\sum_{\mu=2}^{\infty}\frac{1}{(\mu!)^2}\sum_{i_1\neq i_2\neq\cdots\neq i_{2\mu}} b_{i_1}^{\dagger} b_{i_2}^{\dagger}\cdots b_{i_\mu}^{\dagger}\times b_{i_{\mu+1}} b_{i_{\mu+2}}\cdots b_{i_{2\mu}}\ , \tag{1}$$

where p is the total number of Nilsson levels (orbits) considered, where $G>0$ is the overall pairing strength, ϵ_i are the single-particle energies obtained in the Nilsson model, $n_i=a_{i\uparrow}^{\dagger}a_{i\uparrow}+a_{i\downarrow}^{\dagger}a_{i\downarrow}$ is the fermion number operator for the i-th Nilsson level, and $b_i^{\dagger}=a_{i\uparrow}^{\dagger}a_{i\downarrow}^{\dagger}$ [$b_i=(b_i^{\dagger})^{\dagger}=a_{i\uparrow}a_{i\downarrow}$] are pair creation [annihilation] operators. The up and down arrows in these expressions refer to time-reversed states. Let $|i_1,\ldots,i_m\rangle$ be the pairing vacuum state that satisfies

$$b_i|i_1,\ldots,i_m\rangle=0 \tag{2}$$

for $1\le i\le p$, where each of the m levels, $i_1,i_2,\ldots,i_m$, is occupied by a single nucleon. Following the algebraic Bethe ansatz used in Ref. [19], one can write a k-pair eigenstate as

$$|k;\zeta;i_1,\ldots,i_m\rangle = \sum_{1\leqslant i_1<\cdots<i_k\leqslant p} C^{(\zeta)}_{i_1 i_2\cdots i_k} b_{i_1}^{\dagger} b_{i_2}^{\dagger}\cdots b_{i_k}^{\dagger}|i_1,\ldots,i_m\rangle\ , \tag{3}$$

where $C^{(\zeta)}_{i_1 i_2\cdots i_k}$ are expansion coefficients that need to be determined. It is assumed that the levels i_1, i_2, …, i_m should be excluded from the summation in Eq. (3). The expansion coefficient $C^{(\zeta)}_{i_1 i_2\cdots i_k}$ can be expressed very simply as

$$C^{(\zeta)}_{i_1 i_2\cdots i_k}=\frac{1}{1-\chi^{(\zeta)}\sum_{\mu=1}^{k}\epsilon_{i_\mu}}\ , \tag{4}$$

where $\chi^{(\zeta)}$ is a parameter that needs to be determined. The k-pair eigenenergies of Eq. (1) are given by

$$E_k^{(\zeta)}=\frac{2}{\chi^{(\zeta)}}-G(k-1)\ , \tag{5}$$

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

$$\frac{2}{\chi^{(\zeta)}}+\sum_{1\leqslant i_1<i_2<\cdots<i_k\leqslant p}\frac{G}{(1-\chi^{(\zeta)}\sum_{\mu=1}^{k}\epsilon_{i_\mu})}=0\ , \tag{6}$$

in which $\chi^{(\zeta)}$ is the ζ-th solution of Eq. (6). Similar results for even-odd systems can also be derived by using this approach except that the index i of the level occupied by the single nucleon should be excluded from the summation Eq. (4) and the single-particle energy ϵ_i contributing to the eigenenergy from the first term of Eq. (2) should be included in Eq. (8). Extensions to many broken-pair cases are thus straightforward.

3 The ground state occupation probabilities of valence nucleon pairs

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,

$$b_i^{\dagger}=\sum_{j_i j_i'} W^i_{j_i} W^i_{j_i'}(-)^{j_i'-\Omega_i} c^{\dagger}_{j_i\Omega_i} c^{\dagger}_{j_i'\ \overline{\Omega}_i}, \tag{7}$$

where $c^{\dagger}_{j_i\Omega_i}$ is the single-particle creation operators with definite angular momentum quantum number j_i, Ω_i is the projection of j_i onto the third axis of the intrinsic frame, and $W^i_{j_i}$, are normalized expansion coefficients of the i-th Nilsson state expanded in terms of a set of spherical shell model states. In addition,

$$c^{\dagger}_{j_i\Omega_i} c^{\dagger}_{j_i'\overline{\Omega}_i}=\sum_{J_i}\langle j_i\Omega_i j_i'\overline{\Omega}_i|J_i 0\rangle B^{\dagger}_{j_i j_i' J_i 0}\ , \tag{8}$$

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 quantum number J_i. Thus, we also have

$$B^{\dagger}_{j_i j_i' J_i 0}=\sum_{j_i j_i'}\langle j_i\Omega_i j_i'\overline{\Omega}|J_i 0\rangle c^{\dagger}_{j_i\Omega_i} c^{\dagger}_{j_i'\overline{\Omega}_i}\ . \tag{9}$$

By substituting Eq. (8) into Eq. (7), Eq. (7) becomes

$$b_i^{\dagger}=\sum_{j_i j_i'} W^i_{j_i} W^i_{j_i'}(-)^{j_i'-\Omega_i}\sum_{J_i}\langle j_i\Omega_i j_i'\overline{\Omega}_i|J_i 0\rangle B^{\dagger}_{j_i j_i' J_i 0}\ . \tag{10}$$

By substituting Eq. (10) into Eq. (3), the k^ρ-pair eigenstates of the model can be expressed as

$$|k^\rho;\ \zeta;\ 0\rangle = \sum_{1\le i_1<\cdots<i_k\le p} C^{(\zeta)}_{i_1 i_2\cdots i_k} \prod_{i=1}^{k^\rho} \left(\sum_{j_i j_i'} W^i_{j_i} W^i_{j_i'} (-)^{j_i'-\Omega_i} \sum_{J_i} \langle j_i \Omega_i j_i' \overline{\Omega}_i | J_i 0\rangle B^\dagger_{j_i j_i' J_i 0}(\rho) \right) |0\rangle\ , \tag{11}$$

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

$$n^\rho_J = \langle k^\rho;\ \zeta=1;\ 0| \sum_{jj'} B^\dagger_{jj'J0}(\rho) \frac{\partial}{\partial B^\dagger_{jj'J0}(\rho)} |k^\rho;\ \zeta=1;\ 0\rangle\ , \tag{12}$$

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

$$\eta_J = \frac{n^\pi_J + n^\nu_J}{k}\ , \tag{13}$$

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

4 Even-odd mass differences

The even-odd mass differences $P(A)$ of the three chains of isotopes are calculated for which both the valence neutron and proton sectors are taken into account. The deformation parameters ε_2 are extracted from the experimental data[20]. The pairing interaction strength G used here is obtained from the results shown in Ref. [18], which are determined by fitting the experimental values of the binding energies, the odd-even mass differences, and the experimental value of the first pairing excitation energies in the extended pairing model. The odd-even mass differences defined by $P(Z,N)=E_B(Z,N+1)+E_B(Z,N-1)-2E_B(Z,N)$, where $E_B(Z,N)$ is the binding energy of a nucleus with proton number Z and neutron number N, are calculated from the model for the Er, Yb, and Hf isotopes. These quantities are more sensitive to pairing correlations as compared to binding energies. As shown in Fig. 1, the even-odd mass differences of the three chains of isotopes are very close to the corresponding experimental data[20].

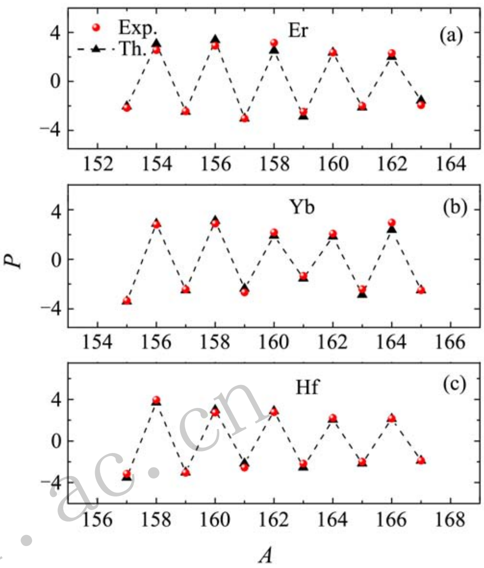

Fig. 1 (color online) Theoretical and experimental even-odd mass differences (in MeV) for $^{153-163}$Er, $^{155-165}$Yb, and $^{157-167}$Hf. Experimental values are denoted as "Exp.", and theoretical values calculated in the extended pairing model are denoted as "Th.".

5 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 $^{157-164}$Yb in the framework of the extended pairing model are also calculated. According to the Inglis cranking formula[21], the moment of inertia of a nucleus is calculated by

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

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 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 Eq. (14) is negligible[22].

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 Ω satisfies $\Delta I = 1$ in ^{161}Yb, of which the experimental value of the moment of inertia is obtained according to Ref. [18], while the difference of the spins of adjacent levels in the ground-state band with bandhead spin Ω satisfies $\Delta I = 2$ in ^{163,165}Yb, of which the experimental values of the moments of inertia are obtained according to Ref. [18]. The level energies of these isotopes are all taken form Ref. [23]. For ^{157}Yb and ^{159}Yb, the total spin I of the first excited state in the ground-state band is also not observed experimentally. Hence, the experimental moments of inertia of ^{157}Yb and ^{159}Yb are absent.

The calculated moments of inertia and the corresponding experimental data for the even-even nuclei in the three isotopic chains are shown in Fig. 2. 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[24, 25].

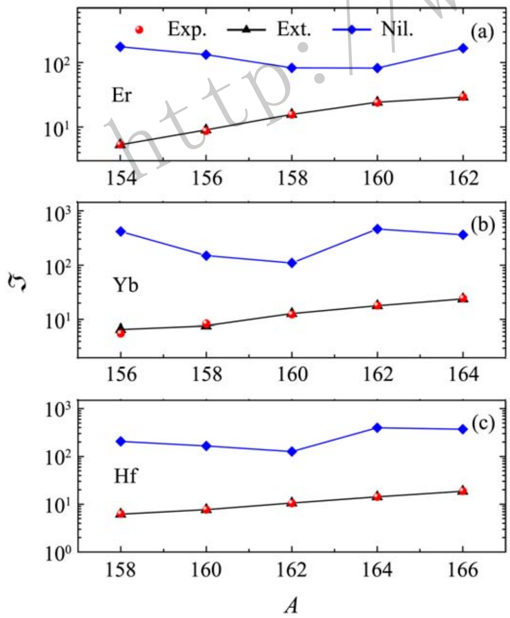

Fig. 2 (color online) Theoretical and experimentally deduced values of the moment of inertia in $\hbar^2(\mathrm{MeV})^{-1}$ for even-even $^{154-162}$Er, $^{156-164}$Yb, and $^{158-166}$Hf, where "Ext." denotes theoretical results obtained in the extended pairing model, "Nil." denotes theoretical results obtained in the Nilsson mean field without pairing interaction, and the values denoted by "Exp." are extracted from the experimental spectra of these nuclei[23].

Similar to the definition of the odd-even mass difference, the relative odd-even difference of the moments of inertia may be defined as[25]

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

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. 3(a). The relative odd-even differences of the moments of inertia $P_{\Im}$ for Yb are shown in Fig. 3(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.

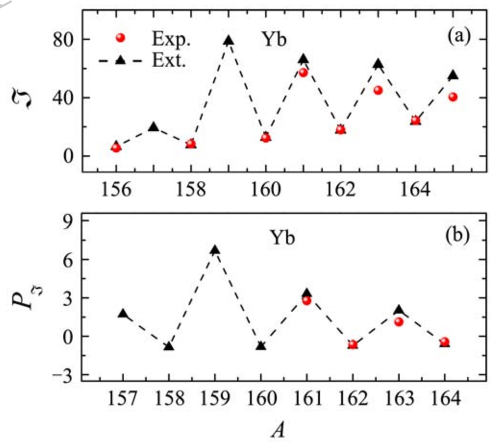

Fig. 3 (color online) (a) Theoretical and experimentally deduced moments of inertia in $\hbar^2(\mathrm{MeV})^{-1}$ for $^{156-165}$Yb, where "Ext." denotes results obtained in the extended pairing model, and "Exp." denotes the corresponding values extracted from the experimental spectra of these nuclei[23]. (b) Relative even-odd differences of the moments of inertia of $^{157-164}$Yb, calculated by Eq. (15), where experimental data is denoted by "Exp." and and theoretical values in the extended pairing model, are denoted as "Ext.".

6 Ground state occupation probabilities of valence nucleon pairs with various angular momentum quantum numbers

Firstly, as an realistic example, we consider the neutron part of ^{158}Yb described in the model with

$p = 22$ Nilsson levels and $k^{\nu}=3$ valence neutron pairs, of which the deformation parameter $\varepsilon_2 = 0.15$ is extracted from experimental data[20]. As has shown in Ref. [18], by fitting the experimental values of the binding energies, the odd-even mass differences, and the experimental value of the first pairing excitation energies, the neutron pairing interaction strength $G^{\nu} = 0.0127$ MeV in the extended pairing model is thus determined. As shown in Fig. 4, it is obvious that the occupation probability of valence nucleon pairs with angular momentum quantum number J decreases with the increasing of J, in which those of even-J pairs are much higher than those of odd-J pairs. Moreover, among the occupation probabilities of even-J pairs, those with $J=0$, 2, 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 and the weight of angular momenta $J=4$ to $J=10$ are comparable with the lower S and D ones.

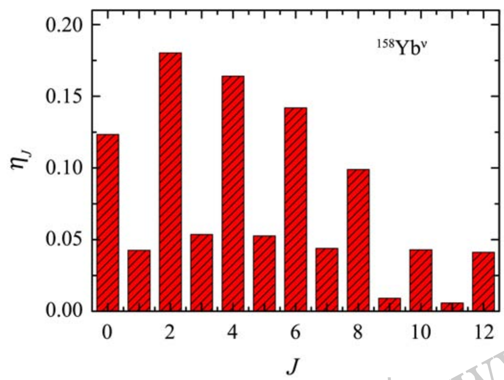

Fig. 4 (color online) Ground state occupation probabilities of valence neutron pairs with angular momentum quantum number J in ^{158}Yb ($k^{\nu}=3$) calculated in the model.

Secondly, we study the ground state occupation probabilities of valence nucleon pairs with angular momentum quantum number J in $^{156-162}$Yb isotopes, for which both the valence neutron and proton sectors are taken into account. The deformation parameters ε_2 are extracted from the experimental data[20]. The pairing interaction strength G used here is obtained from the results shown in Ref. [18], which are determined by fitting the experimental values of the binding energies, the odd-even mass differences, and the experimental value of the first pairing excitation energies in the extended pairing model. Fig. 5 displays the calculated results for the ground state occupation probabilities of valence nucleon pairs with $J = 0$ to $J = 12$ for $^{156-162}$Yb. It is obvious that the occupation probability decreases with the increasing of J, in which those of even-J pairs are much higher than those of odd-J pairs. Moreover, among the occupation probabilities of even-J pairs, those with $J = 0$, 2, 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. Particularly, the above conclusions are independent of the mass number A. For ^{156}Yb, the occupation probability of $J = 0$ pairs is close to that of $J=2$ pairs and a little higher than

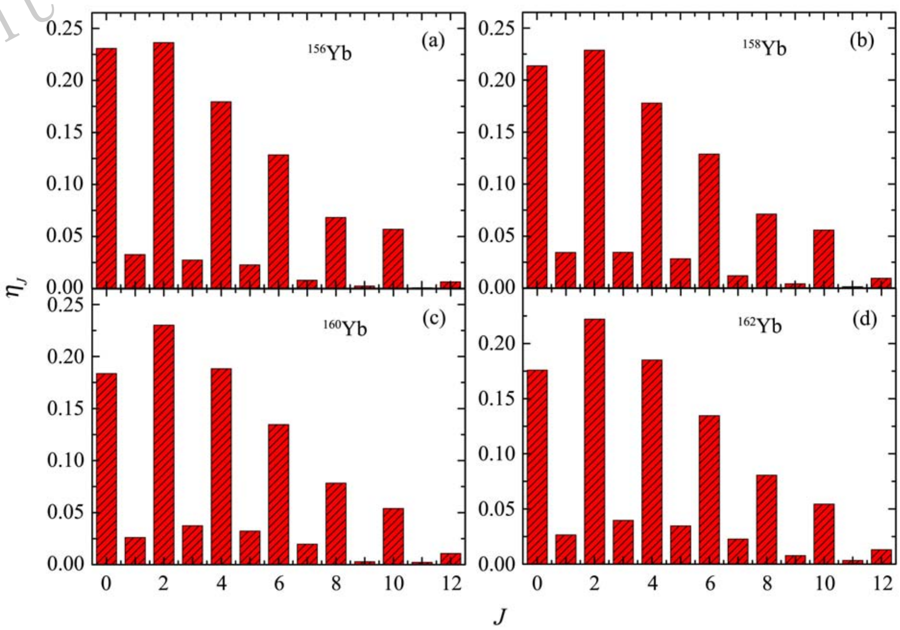

Fig. 5 (color online) Ground state occupation probabilities of valence nucleon pairs with angular momentum quantum number J in $^{156-162}$Yb calculated in the Nilsson mean-field plus the extended-pairing model.

that of $J = 4$ pairs. With the increasing the mass number A, the occupation probability of $J = 0$ pairs becomes lower. Especially, as shown in Fig. 5, the occupation probability of $J = 0$ pairs is lower than that of $J = 2$ and $J = 4$ pairs in ^{162}Yb.

7 Conclusions

In summary, the Nilsson mean-field plus extended-pairing model for well-deformed nuclei is applied to describe rare earth nuclei. Binding energies, even-odd mass differences, and moments of inertia of $^{152-164}$Er, $^{154-166}$Yb, and $^{156-168}$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.

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 G pairs 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 $^{156-162}$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. [14], 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 Refs. [26, 27]. 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 angular momentum projection technique, which will be a part of our future work.

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Er, Yb 和 Hf 同位素的基态占有率

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摘要: 应用严格求解的 Nilsson 平均场加推广对力模型，在同时考虑质子-质子和中子-中子间对力相互作用的情况下，对稀土区的 $^{152-164}$Er, $^{154-166}$Yb 和 $^{156-168}$Hf 核素的结合能、奇偶能差、低激发态转动惯量等基态性质进行系统的统一描述。通过计算结果与实验数值比较分析显示，对力相互作用在阐明以上核素能谱的基态性质中起到了关键的作用。应用拟合上述物理量所确定的模型参数，对 $^{156-162}$Yb 核素基态中价核子配成角动量 $J=0,1,\cdots,12$ 的价核子对占有率的计算结果显示，配成角动量为偶数价核子对的占有率远远高于配成角动量为奇数价核子对的占有率，其数值结果揭示了配成角动量为 S, D 和 G 的价核子对在所考虑的核素基态性质中占主导地位。

关键词: 基态占有率；对力强度；Nilsson 平均场加推广对力模型

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