Nilsson mean-field plus the extended pairing model description of rare earth nuclei*

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Abstract: The Nilsson mean-field plus the extended pairing model for well-deformed nuclei is applied to some representative rare earth examples. The binding energies, some low-lying pair-excited states and even-odd mass differences of Er, Yb and Hf isotopes are calculated systematically within the proton frozen-pair excitation limit. A comparison with experimental data for these nuclei shows that the results of the extended pairing model are better than those for the standard pairing model with the BCS approximation and the nearest-orbit pairing model.

Key words: Nilsson mean-field, pairing interaction, binding energy, even-odd mass difference

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1 Introduction

Besides the quadrupole-quadrupole interaction, pairing is an important residual interaction in nuclei. The Bardeen-Cooper-Schrieffer (BCS) and Hartree-Fock-Bogolyubov (HFB) methods [1, 2] for finding approximate solutions are well known. However, both the BCS and HFB approximations suffer from serious drawbacks. The nonconservation of the number of particles is one that can lead to serious problems, such as spurious states, nonorthogonal solutions, etc. Another problem with approximate treatments of the pairing Hamiltonian is related to the fact that both the BCS and the HFB approximations break down for an important class of physical situations. The often proposed particle-number projection remedy complicates the algorithms considerably and usually without yielding a better description of higher-lying excited states that are a natural part of the spectrum of the pairing Hamiltonian [3–5].

The Nilsson mean-field plus the extended pairing model was introduced to address this challenge and provide a better description of well-deformed nuclei [6]. The advantage of the model is that it is exactly solvable and that the number of valence pairs is a conserved quantity. In addition, as shown in our recent study [7], the extended pairing model is equivalent to the conventional standard pairing Hamiltonian within the first step of the approximation, which displays the pair structures of low-lying states of the standard pairing model. Moreover, the nearest orbit pairing model [8], which is a simplified version of the Gaussian type of pairing interaction suitable for describing well-deformed nuclei [5], was also simply solvable with pair-number conserved solutions.

In summary, in this paper we report on an application of the extended pairing model to nuclei in the rare earth region, with a comparison of the results with those from an application of the standard pairing model and the nearest orbit pairing model. The comparison affirms the applicability of the extended pairing model in this region of deformed nuclei.

2 The extended pairing model

The standard pairing Hamiltonian for well-defor-

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med nuclei is given by

$$\hat{H}=\sum_{j=1}^{p}\epsilon_j n_j - G\sum_{i,j=1}^{p} a_i^+ a_j, \tag{1}$$

where p is the total number of Nilsson levels considered, $G>0$ is the overall pairing strength, ϵ_j is the single-particle energies taken from the Nilsson model, $n_j=c_{j\uparrow}^\dagger c_{j\uparrow}+c_{j\downarrow}^\dagger c_{j\downarrow}$ is the fermion number operator for the j-th Nilsson level and $a_i^+=c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$ $[a_i=(a_i^+)^\dagger=c_{i\downarrow}c_{i\uparrow}]$ are pair creation [annihilation] operators. The up and down arrows in these expressions refer to time-reversed states.

Since it is not possible to diagonalize Hamiltonian (1) in a large Fock subspace, the BCS approximation is often invoked. As an alternative approach, the extended pairing model was proposed [6] with the Hamiltonian:

$$\hat{H}=\sum_{j=1}^{p}\epsilon_j n_j - G_{\rm ep}\sum_{i,j=1}^{p} a_i^+ a_j - G_{\rm ep}\left(\sum_{\mu=2}^{\infty}\frac{1}{(\mu!)^2}\times\sum_{i_1\neq i_2\neq\cdots\neq i_{2\mu}} a_{i_1}^+ a_{i_2}^+\cdots a_{i_\mu}^+ a_{i_{\mu+1}}a_{i_{\mu+2}}\cdots a_{i_{2\mu}}\right), \tag{2}$$

where no pair of indices among $\{i_1,i_2,\cdots,i_{2\mu}\}$ is the same for any μ. Besides the usual 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. With this extension in play, the model becomes exactly solvable.

The k-pair excitation energies of (2) are given by

$$E_k^{(\zeta)}=\frac{2}{\chi^{(\zeta)}}-G_{\rm ep}(k-1), \tag{3}$$

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

$$\frac{2}{\chi^{(\zeta)}}+\sum_{1\leqslant i_1<i_2<\cdots<i_k\leqslant p}\frac{G_{\rm ep}}{(1-\chi^{(\zeta)}\sum_{\mu=1}^{k}\epsilon_{i_\mu})}=0, \tag{4}$$

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

In any mean-field plus pairing model, the binding energy can be calculated in the following way: (a) For a chain of isotopes, the number of valence protons is a constant. Hence, the contribution from valence protons to binding energy is also a constant. Therefore, only the neutron Hamiltonian given by (2) needs to be considered. As a consequence, contributions to excitation energies from the proton pairing interaction can be ignored, which is called the frozen proton-pair excitation approximation. (b) Since only the valence neutrons above a major shell are considered, the contributions to the binding energy from the core are roughly constant and can be simply added in without affecting the excitation spectra. Furthermore, besides the residual interactions among valence neutrons, the binding energy also increases with increasing the number of valence particles and this is many orders of magnitude larger than that due to the residual pairing, which can be estimated from the binding energy per particle of the nucleus. As a consequence, in the calculation, the neutron single-particle energy is expressed as $\epsilon_j=\overline{\epsilon}_j-\epsilon_0-\epsilon$, where $\overline{\epsilon}_j$ is the neutron single-particle energy calculated from the Nilsson model, ϵ_0 is the contribution from the core, which can be determined by the corresponding magic nucleus in the beginning of a major shell being considered and ϵ is the average binding energy per valence neutron in the shell and is taken to be a parameter of the theory. In the rare earth region, for example, since the valence neutrons (protons) occupy Nilsson orbits in the sixth (fifth) major shell, ϵ_0 for the neutron (proton) single-particle energy is just the single-particle energy of the last Nilsson level for neutrons (protons) of ^{132}Sn, while the average binding energy per valence neutron in the sixth major shell ϵ is a parameter that is adjusted to fit the binding energy, and as an approximation, taken to be a constant for the entire shell. Since only one major shell is considered and there are 22 Nilsson levels in the sixth major shell, the total number of Nilsson orbits is $p=22$ for the valence neutrons in our calculation. Finally, the binding energy of nuclei in the rare earth region can be expressed as

$$E_{\rm B}=E_{\rm B}^{(\rm core)}+E_{\rm B}(\pi)+E_{\rm B}(\nu), \tag{5}$$

where $E_{\rm B}^{(\rm core)}$ is the binding energy of ^{132}Sn, $E_{\rm B}(\pi)$ is the binding energy contributed from the mean-field plus pairing interaction among the valence protons, which is approximately a constant because the number of valence protons is fixed for a chain of isotopes and $E_{\rm B}(\nu)$ is the binding energy contributed from the mean-field plus pairing interaction of the valence neutrons calculated from (1) in the standard pairing model, from (2) in the extended pairing model and from the corresponding Hamiltonian of the nearest orbit pairing model [8]. Deformation parameters of the Nilsson mean-field for all isotopes considered are taken from [9], which were determined systematically from the corresponding experimental data [10].

3 Numerical results and discussions

In the rare earth region, the experimental data on Er, Yb and Hf isotopes are more abundant than for most other isotopes and therefore these were chosen for this study. The binding energies, even-odd mass differences and pairing excitation energies were fit by the Nilsson mean-field plus the extended pairing model and compared with the results obtained from the standard pairing and nearest orbit pairing models. We used a mean-square deviation measure to estimate the deviation of binding energies in a chain of isotopes with

$$\sigma = \left[\sum_{\mu}(E_{\mu}^{\rm th} - E_{\mu}^{\rm exp})^2/\mathcal{N}\right]^{\frac{1}{2}}, \qquad (6)$$

where $E_{\mu}^{\rm th}$ is the theoretical value of the binding energy, $E_{\mu}^{\rm exp}$ is the corresponding experimental value, $\mathcal{N}$ is the total number of nuclei considered and the sum runs over the nuclei in the chain.

In the fitting procedure, the average binding energy per particle ϵ and the pairing interaction strength parameters were determined from the corresponding experimental values for the binding energies of the isotopes considered. In the extended pairing model, for example, the best fit requires that $\epsilon = -7.475$ MeV for the Er isotopes, $\epsilon = -7.476$ MeV for the Yb isotopes and $\epsilon = -7.71$ MeV for the Hf isotopes. Specifically, for ^{160}Er, $G_{\rm ep} = 0.001205$ MeV in the extended pairing model, while $G = 0.055$ MeV in the standard pairing model with BCS approximation. In the nearest orbit pairing model, the nearest orbit pairing parameters are $G_{\alpha\beta} = A{\rm e}^{-B(\epsilon_\alpha - \epsilon_\beta)^2}$ when α and β are the same or the nearest orbits, where ϵ_α is the single particle energy of the orbit α obtained from the Nilsson model [5]. In this case, the parameters $A = 2.33$ MeV, $B = 0.1$ MeV^{-2} for ^{160}Er. Once the binding energies are fit, the even-odd mass difference is calculated from

$$P(A) = E_{\rm B}(A+1) + E_{\rm B}(A-1) - 2E_{\rm B}(A), \qquad (7)$$

where $E_{\rm B}(A)$ is the binding energy of a nucleus with mass number A.

The quality of the fits, as measured by mean-square deviation from experiment, of the extended pairing (EP) model, the standard pairing model enha-

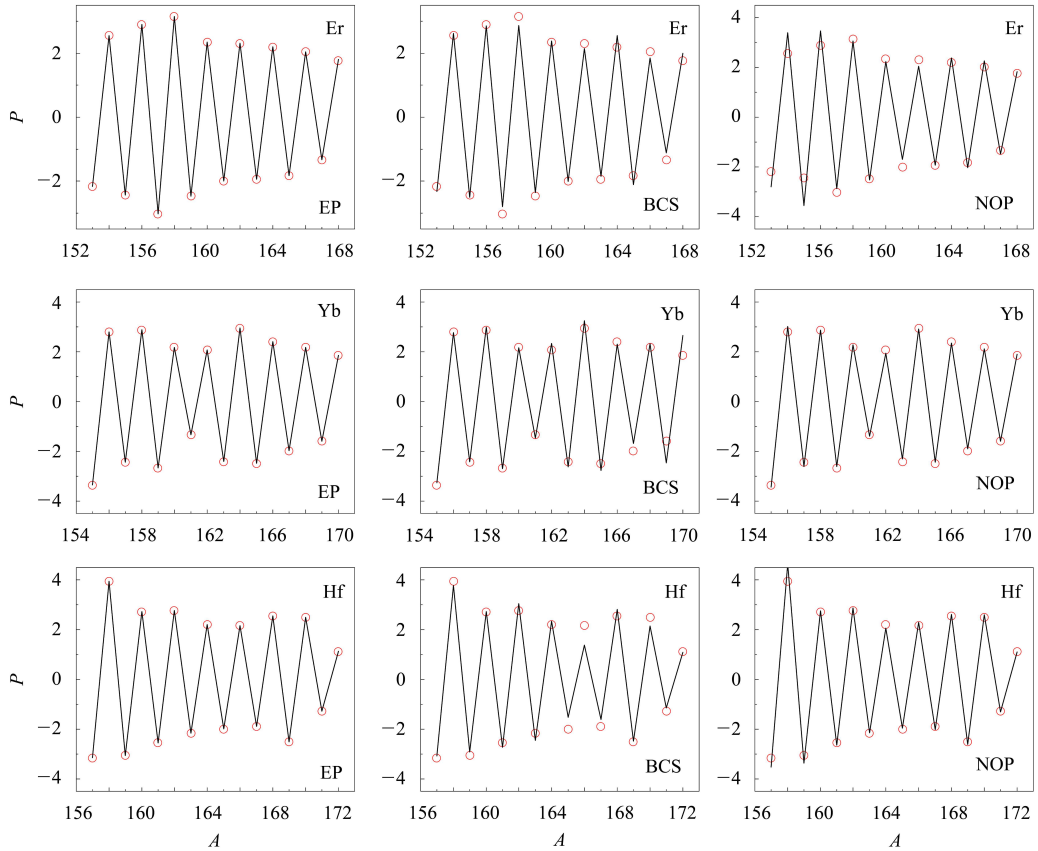

Fig. 1. The theoretical values and the corresponding experimental values [10] of the even-odd mass differences of $^{154-169}$Er, $^{156-171}$Yb and $^{156-173}$Hf, where P (in MeV) is the even-odd mass difference, A is the mass number of the nucleus, the dots show the experimental values and the theoretical values are connected by the lines.

nced by the BCS approximation and a nearest orbit pairing (NOP) model, are shown in Table 1. These results very clearly demonstrate that for the nuclei considered, the extended pairing model reproduces binding energies considerably closer to experiment than the other two models. Fig. 1 also shows the even-odd mass differences among the nuclei in these isotopic chains. The latter is a further, even more stringent test of the applicability of each model. So, although the three models produce generally similar results, these analyses suggest that the extended pairing model with deviations as shown in Table 1 is a better description for the nuclei of Fig. 1.

Table 1. The mean-square deviation (in MeV) for fits to the binding energies of $^{154-169}$Er, $^{156-171}$Yb and $^{156-173}$Hf.

nucleus	$\sigma_{\rm EP}$	$\sigma_{\rm BCS}$	$\sigma_{\rm NOP}$
Er	0.0095	0.0824	0.1634
Yb	0.0003	0.1205	0.0419
Hf	0.0001	0.1163	0.0957

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 these models can be regarded approximately as pairing excitation states with the same spin and parity as those of the ground state of a nucleus. Table 2 provides the pairing excitation energies obtained from the extended pairing model, $E_{\rm EP}$, the nearest orbit pairing model, $E_{\rm NOP}$ and the standard pairing model with BCS approximation, $E_{\rm BCS}$, in comparison with those observed in experiment. Some deviation from the experimental data is expected since the proton pairing excitation is frozen and the proton-neutron quadrupole-quadrupole interaction is neglected. Nevertheless, the comparisons are not unreasonable, with the extended pairing model typically showing better results – in most cases – than the other models.

Table 2. The pairing excitation energies (in MeV) of $^{166-173}$Hf, $^{154-169}$Er, and $^{160-171}$Yb, where $E_{\rm EP}$ is the pairing excitation energy calculated from the extended pairing model, $E_{\rm NOP}$ is that calculated from the nearest orbit pairing model, $E_{\rm BCS}$ is that calculated from the standard pairing model with BCS proximation and the experimental data are taken from Ref. [11]. The dash denotes that the corresponding state is not observed in experiment.

nucleus	mass number	spin and parity	$E^{\rm exp}$	$E_{\rm EP}$	$E_{\rm NOP}$	$E_{\rm BCS}$
$^{166-173}$Hf	166	0_2^+	0.695	0.726	0.651	0.333
		0_3^+	0.909	1.163	1.333	1.304
	167	$\frac{5}{2}{}_2^-$	——	0.528	0.876	1.109
		$\frac{5}{2}{}_3^-$	——	0.883	1.793	1.998
	168	0_2^+	0.942	1.111	0.691	0.932
		0_3^+	——	1.995	1.332	1.752
	169	$\frac{5}{2}{}_2^-$	0.059	0.179	0.872	0.902
		$\frac{5}{2}{}_3^-$	——	0.411	0.879	1.381
	170	0_2^+	0.880	0.721	0.6772	0.834
		0_3^+	——	1.633	1.428	1.304
	171	$\frac{7}{2}{}_2^+$	0.555	0.134	0.800	0.837
		$\frac{7}{2}{}_3^+$	0.789	0.729	0.972	1.445
	172	0_2^+	0.871	0.799	0.645	0.608
		0_3^+	1.295	0.867	1.647	0.725
	173	$\frac{1}{2}{}_2^-$	——	0.041	0.416	0.066
		$\frac{1}{2}{}_3^-$	——	0.632	1.609	1.026
$^{154-169}$Er	154	0_2^+	——	0.893	1.114	0.236
		0_3^+	——	1.587	2.264	1.482
	155	$\frac{7}{2}{}_2^-$	——	0.368	1.264	0.313
		$\frac{7}{2}{}_3^-$	——	0.543	2.828	1.697
	156	0_2^+	0.9304	0.850	1.305	1.201
		0_3^+	——	2.040	2.240	1.522
	157	$\frac{3}{2}{}_2^-$	0.110	1.031	1.789	0.351
		$\frac{3}{2}{}_3^-$	0.242	1.352	2.048	0.981

Table 2. (continued)

nucleus	mass number	spin and parity	$E^{\rm exp}$	$E_{\rm EP}$	$E_{\rm NOP}$	$E_{\rm BCS}$
$^{154-169}$Er	158	0_2^+	0.806	1.087	1.083	0.238
		0_3^+	1.387	1.364	1.893	0.864
	159	$\frac{3}{2}^-_2$	——	0.914	0.587	0.090
		$\frac{3}{2}^-_3$	——	0.897	1.231	0.950
	160	0_2^+	0.894	0.891	0.9623	0.041
		0_3^+	——	0.967	1.794	0.922
	161	$\frac{3}{2}^-_2$	0.725	0.292	1.016	0.925
		$\frac{3}{2}^-_3$	——	0.397	2.235	1.496
	162	0_2^+	1.087	0.854	0.923	0.827
		0_3^+	1.421	1.901	1.877	1.447
	163	$\frac{5}{2}^-_2$	0.164	0.164	1.027	1.432
		$\frac{5}{2}^-_3$	0.440	0.604	1.935	2.769
	164	0_2^+	1.246	1.514	0.991	0.796
		0_3^+	1.417	2.459	1.913	2.004
	165	$\frac{5}{2}^-_2$	0.296	0.096	1.612	1.252
		$\frac{5}{2}^-_3$	0.384	0.397	2.131	1.989
	166	0_2^+	1.460	1.813	0.942	1.182
		0_3^+	2.189	3.083	1.559	1.915
	167	$\frac{7}{2}^-_2$	0.641	0.134	1.471	1.161
		$\frac{7}{2}^-_3$	0.873	0.809	1.589	2.065
	168	0_2^+	1.217	1.915	0.695	1.299
		0_3^+	1.422	5.255	1.289	1.423
	169	$\frac{1}{2}^-_2$	0.562	0.561	1.023	0.415
		$\frac{1}{2}^-_3$	1.094	4.381	1.530	0.973
$^{160-171}$Yb	160	0_2^+	1.086	0.659	0.851	0.448
		0_3^+	——	1.497	1.476	0.756
	161	$\frac{3}{2}^-_2$	0.211	0.147	1.095	0.748
		$\frac{3}{2}^-_3$	——	0.371	1.236	0.804
	162	0_2^+	0.606	1.815	0.548	0.654
		0_3^+	1.006	2.638	1.465	0.662
	163	$\frac{3}{2}^-_2$	0.871	0.388	0.981	0.535
		$\frac{3}{2}^-_3$	——	0.511	2.066	1.471
	164	0_2^+	0.976	1.777	0.867	0.268
		0_3^+	——	2.150	1.736	1.186
	165	$\frac{5}{2}^-_2$	0.174	0.469	0.759	1.273
		$\frac{5}{2}^-_3$	0.401	1.427	1.279	2.397
	166	0_2^+	1.043	1.590	0.944	0.852
		0_3^+	——	2.715	1.788	1.846
	167	$\frac{5}{2}^-_2$	0.278	0.121	1.179	0.992
		$\frac{5}{2}^-_3$	0.239	0.369	2.444	1.513
	168	0_2^+	1.154	2.063	0.887	0.941
		0_3^+	1.197	3.190	1.630	1.612
	169	$\frac{7}{2}^+_2$	0.647	0.133	0.713	0.988
		$\frac{7}{2}^+_3$	0.832	1.064	1.605	1.825
	170	0_2^+	1.069	1.851	0.812	0.772
		0_3^+	1.229	2.167	1.350	0.844
	171	$\frac{1}{2}^-_2$	0.953	0.698	1.042	0.788
		$\frac{1}{2}^-_3$	0.988	1.148	1.298	0.862

4 Summary

The mean-field plus the extended pairing model for well-deformed nuclei is used to describe the rare earth nuclei. Within the proton frozen-pair approximation, the binding energies, pairing excitation energies, even-odd mass differences of some Er, Yb and Hf isotopes are calculated and compared with the corresponding experimental data, the results obtained from the standard pairing model with BCS approximation and the nearest orbit pairing model. The results show that the extended pairing model is systematically better than the other two models in fits within these three chains of isotopes as far as the binding energies and even-odd mass differences are considered. However, the deviation in pairing excitation energies is less well described, presumably due to the proton frozen-pair approximation and the negligence of proton-neutron quadrupole-quadrupole interaction. Further analyses along this line are in progress. An extension that adopts a relativistic mean-field [12] plus the extended pairing interaction is straightforward and will be presented elsewhere. Since the total angular momentum in these deformed mean-field plus the pairing models is not a conserved quantity, to study the excited states in these models, an angular momentum projection technique similar to [13] must be adopted. Work related to this is also in progress.

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