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Ground State Shape (Phase) Crossover in Er and Yb Isotopes

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Abstract: Ground-state shape (phase) crossover in Er and Yb isotopes is manifested in the axially deformed Nilsson mean-field plus extended pairing model. The energy ratio $R_{0_2^+/2_1^+}$, the odd-even mass differences and the information entropy are calculated under the present model, reproduce the shape (phase) crossover behaviors of these quantities in $^{155-163}\text{Er}$ and $^{157-165}\text{Yb}$ isotopes. From the analysis of these quantities as functions of the quadrupole deformation parameter and the overall pairing interaction strength, it is shown that the crossover is mainly driven by the competition between the pairing interaction and the quadrupole deformation, which thus provides the origin of the shape (phase) crossover in the present model.

Key words: pairing interaction; crossover; energy ratio

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1 Introduction

Shape phase transitions which occur at zero temperature may be manifested by a sudden change or a crossover of the ground-state structure at a certain critical value of the control parameter, it has been analyzed extensively in both experiment and theory^[1]. These studies have provided new insights into understanding the evolution of nuclear structures, which can be related to different geometrical shapes in nuclei^[2]. In atomic nuclei, quantum phase is often referred to as the shape (phase) of a nucleus. Typical shape is of spherical (vibrational), indefinite triaxial (γ -unstable), or axially deformed (rotational) type, which is manifested by the collective model^[3] and the interacting boson model (IBM)^[4]. Shape (phase) crossover can be observed at ground-state or low-lying states of nuclei along a chain of isotopes or isotones, in which noticeable changes in physical quantities or called effective order parameters, such as energy ratios, $B(E2)$ ratios, and binding energy related quantities, are not only predicted theoretically, but also experimentally observed^[1]. Rigorously speaking, the QPT (Quantum Phase Transitions) should be defined in the thermodynamic or large- N limit. Since the number of nucleon in a nuclear system is always finite, instead of dramatic changes or discontinuity in effective order parameters,

only a crossover with a finite- N effect from one shape to another may be observed, especially at the critical point of the transition^[5].

Recently, it has been experimentally observed that the odd-even mass difference and some mass related quantities, which are the most significant evidence of pairing interaction, may exhibit critical behavior around the neutron number $N=90$ in $A \sim 150$ mass region^[6-7], of which some relevant quantities can thus be taken as effective order parameters of the evolution from spherical to axially deformed shape (phase). Therefore, the shape (phase) evolution of nuclei in this mass region should suitably be explored by the Nilsson (deformed) mean-field plus pairing model as shown in our previous work^[8-11], with which the nature of the critical behavior of the shape (phase) evolution driven by the competition between the deformation and pairing interaction can be revealed from related effective order parameters. However, the nature of the critical behavior, including the role of the quadrupole deformation, is still far from being clear. Particularly, how the competition between the pairing interaction and the quadrupole deformation relate to the phase transition is yet to be resolved. Therefore, it is important to explore possible microscopic mechanisms with an appropriate pairing model that can account for the ground-state shape phase transition reflected by the

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related odd-even effects in nuclei.

The purpose of this work is to systematically analyze the ground-state shape phase transition in Yb, Er isotopes within the axially deformed Nilsson mean-field plus extended pairing model. The energy ratio $R_{0_2^+/2_1^+}$, odd-even mass differences, and the ground state occupation probabilities of valence nucleon pairs with different angular momenta of these nuclei will be calculated. We examine the effects of both the pairing interaction strength and the quadrupole deformation in the model, from which the role of the pairing interaction and the quadrupole deformation in the shape phase transition in these isotopes will also be addressed.

2 The extended pairing model

The Hamiltonian of the deformed mean-field plus extended pairing model^[8] is given by

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

where p is the total number of Nilsson levels (orbits) considered, $G > 0$ is the overall pairing strength, ϵ_i are the single-particle energies obtained from the axially deformed 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 $b_i^\dagger = a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger$ [$b_i = (b_i^\dagger)^\dagger = a_{i\downarrow} a_{i\uparrow}$] are pair creation [annihilation] operators. The up and down arrows in these expressions refer to time-reversed states. Besides the usual Nilsson mean field and the standard pairing interaction (the first two terms of Eq. (1)), this form includes many-pair hopping terms that allow nucleon pairs to simultaneously scatter (hop) between and among different Nilsson levels. The advantage of the model lies in the fact that it can be solved more easily than the standard pairing model, especially for well-deformed nuclei. Let $|0\rangle$ be the pairing vacuum state that satisfies

$$b_i |0\rangle = 0 \quad (2)$$

for $1 \leq i \leq p$, following the algebraic Bethe ansatz used in Ref. [8], one can write a k -pair eigenstate as

$$|k; \zeta\rangle = \sum_{1 \leq i_1 < \dots < i_k \leq p} C_{i_1 i_2 \dots i_k}^{(\zeta)} b_{i_1}^\dagger b_{i_2}^\dagger \dots b_{i_k}^\dagger |0\rangle, \quad (3)$$

where $C_{i_1 i_2 \dots i_k}^{(\zeta)}$ are expansion coefficients that need to be determined. The expansion coefficient $C_{i_1 i_2 \dots i_k}^{(\zeta)}$ can be expressed very simply as

$$C_{i_1 i_2 \dots i_k}^{(\zeta)} = \frac{1}{1 - \chi^{(\zeta)} \sum_{\mu=1}^k \epsilon_{i_\mu}}, \quad (4)$$

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

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

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

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

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 in Eq. (3) and Eq. (6) and the single-particle energy ϵ_i contributing to the eigenenergy from the first term of Eq. (1) should be included in Eq. (5). Extensions to many broken-pair cases are thus straightforward.

3 The effective order parameter and related quantities

In this section, the energy ratio $R_{0_2^+/2_1^+}$ as a function of the extended pairing interaction strength and the quadrupole deformation parameter of the model is analyzed. The ground-state information entropy are also calculated to reveal the crossover.

As is known in Refs. [12–15], besides the odd-even mass difference, the energy ratio $R_{0_2^+/2_1^+} = (E_{0_2^+} - E_{0_g^+}) / (E_{2_1^+} - E_{0_g^+})$ is also an effective order parameter to reveal the shape (phase) crossover in nuclei, where $E_{0_2^+} - E_{0_g^+}$ is the excitation energy of the second 0^+ state calculated from the present model, and the excitation energy of the first 2^+ state, $E_{2_1^+} - E_{0_g^+}$, of even-even nuclei is obtained according to the energy formula of an axially deformed rotor

$$\frac{2\mathfrak{I}_{\text{th}}}{\hbar^2} = \frac{6}{E_{2_1^+} - E_{0_g^+}}. \quad (7)$$

In Eq. (7), the moment of inertia of the ground band \mathfrak{I}_{th} is calculated in the extended pairing model by using the Inglis cranking formula^[16]

$$\mathfrak{I} = 2\hbar^2 \sum_n \frac{|\langle n | J_{x'} | 0 \rangle|^2}{E_n - E_{0_g^+}}, \quad (8)$$

where $J_{x'}$ is the total angular momentum along the intrinsic x' axis, $|n\rangle$ is the n -th excited state of the extended pairing model, E_n is the corresponding excitation energy, and $E_{0_g^+}$ is the energy of the ground state^[10]. In principle, the summation in Eq. (8) should

run over all excited states. As a good approximation, only one broken-pair states 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 that of the ground state and their contribution to the moment of inertia Eq. (8) is negligible^[17].

In the following, we consider valence neutrons (protons) within the sixth (fifth) major shell with $p = 22$ ($p = 16$) Nilsson levels. In the Nilsson model, only quadrupole deformation is considered with the adjustable quadrupole deformation parameter ε_2 .

Fig. 1 shows the energy ratio $R_{0_2^+/2_1^+}$ as a function of the pairing interaction strength G with a fixed deformation parameter with $\varepsilon_2 = 0.1, 0.125, 0.175$, and 0.25 for $k=3$ neutron pairs over the $p = 22$ Nilsson levels. Those ε_2 values are the typical quadrupole deformation parameter values between 0.1 and 0.25 for the rare earth nuclei which will be studied in the next section. It is clearly shown in Fig. 1 that $R_{0_2^+/2_1^+}$ vary non-monotonically with the increasing of G for all values of ε_2 considered. Particularly, there is a drastic change around $G \sim 0.0078 \sim 0.012$ MeV, which demonstrates the crossover in the present model, namely, the system undergoes the shape (phase) crossover from an axially deformed (rotational) shape with $G=0$ and $R_{0_2^+/2_1^+} \sim 35$ to the spherical (vibrational) shape with sufficiently large G and $R_{0_2^+/2_1^+} \sim 2$ for a given ε_2 studied. The results are quite similar to those of the interacting boson model (IBM) in the $U(5)$ - $SU(3)$ transitional region^[13], in which the energy ratio $R_{0_2^+/2_1^+}$ drops rather precipitously from the rotational limit with $R_{0_2^+/2_1^+} \sim 25$ to the vibrational limit with $R_{0_2^+/2_1^+} \sim 2$.

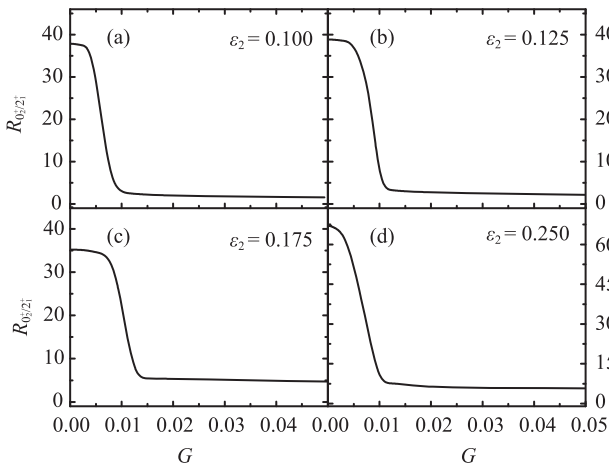


Fig. 1 The energy ratio $R_{0_2^+/2_1^+}$ in the present model for $k=3$ neutron pairs over $p=22$ Nilsson levels as a function of G (in MeV) for several typical values of the deformation parameter ε_2 .

To further explore the nature of the crossover be-

havior in the present model, the information (Shannon) entropy which seems suitable to reveal the crossover due to the results in Refs. [18–19]. The information entropy measures the correlations among the mean-field single-pair product states with k pairs in the ground state $|g\rangle \equiv |k; \zeta = 1; \nu_{j'}\rangle$ of the model, and is defined as

$$I_H(|g\rangle) = - \sum_{i=1}^d |w_i|^2 \log_d(|w_i|^2), \quad (9)$$

where $\{w_i = \langle k|g\rangle\}$ are the expansion coefficients of $|g\rangle$ in terms of the mean-field single-pair product states $|k\rangle$, and d is the dimension of the space spanned by all possible single-pair product states, namely, k pairs distributed over the p levels of the Nilsson mean-field. The information entropy I_H varies within the closed interval $[0, 1]$. $I_H=0$ corresponds to the ground state without the pairing interaction among valence nucleons. In this case, all valence nucleons are in the localized normal state. While $I_H=1$, the pairing interaction is extremely strong leading the ground state to be a valence nucleon-pair condensate, which is referred to as the delocalized superconducting phase. Obviously, the variation of I_H as a function of the pairing interaction strength G for a given value of the deformation parameter sketches the evolution from the localized normal phase towards the delocalized superconducting phase. As shown in Fig. 2, for the same set of values of the deformation parameters ε_2 as that used in Fig. 1, I_H calculated from the present model indicates that the system undergoes the crossover from the localized normal phase with $G=0$ and $I_H=0$ to the delocalized superconducting (pair condensate) phase with sufficiently large G and $I_H \sim 1$. Furthermore, there is also a noticeable change in the information entropy around $G \sim 0.0078 \sim 0.012$ MeV for the four values of the deformation parameter studied as shown in Fig. 2,

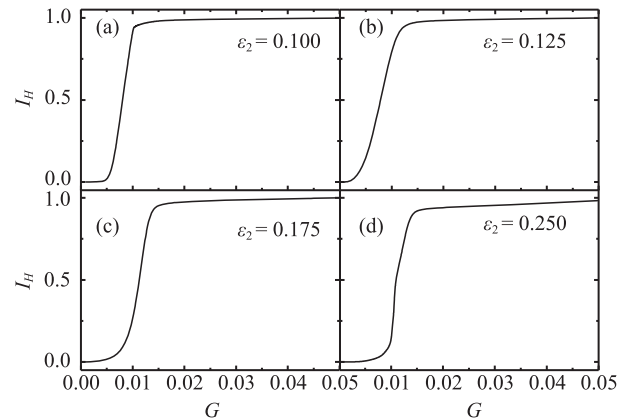


Fig. 2 The information entropy I_H of the ground state as functions of G (in MeV) for the same set of values of the deformation parameter ε_2 as that used in Fig. 3.

which all correspond to the positions where $R_{0_2^+/2_1^+}$ and the occupation probabilities exhibit significant changes as shown Fig. 1. Hence, the crossover behavior shown Fig. 1 is further confirmed. All in all, the ground-state shape (phase) crossover may be driven by the competition between the pairing interaction and quadrupole deformation.

4 Ground state critical behavior in Er and Yb isotopes

In this section, the odd-even mass differences and the energy ratio $R_{0_2^+/2_1^+}$ of $^{154-164}\text{Er}$ and $^{156-164}\text{Yb}$ isotopes will be fitted by using the extended pairing model as examples to reveal the crossover in realistic nuclear systems, in which both valence neutrons and protons are considered explicitly in the model. The deformation parameter ε_2 for each nucleus is extracted from experimental data^[20], which is provided in Table 1. The pairing interaction strength G for each nucleus is determined by fitting the binding energy, the odd-even mass differences, and the first pairing excitation energies in the model^[10], which is shown in Table 2. The pairing interaction strength G for each nucleus is determined by fitting the experimental value of the binding energy, the odd-even mass differences, and the experimental value of the first pairing excitation energies in the extended pairing model^[10]. The odd-even mass difference is defined as $P(Z, N) = E_B(Z, N+1) + E_B(Z, N-1) - 2E_B(Z, N)$, where $E_B(Z, N)$ is the binding energy of a nucleus with proton number Z and neutron number N . As shown in Fig. 3, the theoretical $P(Z, N)$ values are very close to the corresponding experimental data. Moreover, both the theoretical $P(Z, N)$ values as functions of neutron number N and the corresponding experimental values for even-even $^{154-162}\text{Er}$ and $^{156-164}\text{Yb}$ shown in panel (a) of Fig. 3 reach to its maximum at $N=88$. Similar crossover behavior can also be observed in $P(Z, N)$ values for the odd- A case as shown in panel (b), in which $P(Z, N)$ curves have a valley at $N=89$. It is clearly shown that the odd-even mass difference serves as one of the effective order parameters to identify the ground-state crossover^[7, 11].

Moreover, in comparison with the crossover behavior shown in Fig. 1, the two distinguishable phases of the model are the spherical (vibrational) shape (phase) corresponding to $R_{0_2^+/2_1^+} \sim 2$ and the axially deformed (rotational) shape (phase) corresponding to $R_{0_2^+/2_1^+} \sim 35$. Fig. 4 presents both the theoretical and the experimental values of the energy ratio $R_{0_2^+/2_1^+}$ of $^{154-164}\text{Er}$ and $^{156-164}\text{Yb}$. The theoretical $R_{0_2^+/2_1^+}$ values are close to the corresponding experimental values

Table 1 The deformation parameter ε_2 for $^{154-163}\text{Er}$ and $^{156-165}\text{Yb}$ extracted from experimental data^[20].

| Nucleus | ε_2 | Nucleus | ε_2 |
|-------------------|-----------------|-------------------|-----------------|
| ^{154}Er | 0.133 | ^{155}Er | 0.150 |
| ^{156}Er | 0.175 | ^{157}Er | 0.192 |
| ^{158}Er | 0.200 | ^{159}Er | 0.217 |
| ^{160}Er | 0.233 | ^{161}Er | 0.242 |
| ^{162}Er | 0.250 | ^{163}Er | 0.250 |
| ^{156}Yb | 0.117 | ^{157}Yb | 0.142 |
| ^{158}Yb | 0.150 | ^{159}Yb | 0.175 |
| ^{160}Yb | 0.192 | ^{161}Yb | 0.200 |
| ^{162}Yb | 0.208 | ^{163}Yb | 0.225 |
| ^{164}Yb | 0.242 | ^{165}Yb | 0.250 |

Table 2 The neutron (proton) pairing interaction strength G^ν (G^π) (MeV) determined from the binding energies and the odd-even mass differences of $^{154-163}\text{Er}$, $^{156-165}\text{Yb}$.

| Nucleus | G^ν | G^π | Nucleus | G^ν | G^π |
|-------------------|---------|---------|-------------------|---------|---------|
| ^{154}Er | 0.060 0 | 0.009 5 | ^{155}Er | 0.073 0 | 0.009 3 |
| ^{156}Er | 0.012 4 | 0.009 0 | ^{157}Er | 0.012 2 | 0.008 8 |
| ^{158}Er | 0.003 2 | 0.008 5 | ^{159}Er | 0.003 7 | 0.008 2 |
| ^{160}Er | 0.001 1 | 0.008 0 | ^{161}Er | 0.001 4 | 0.007 7 |
| ^{162}Er | 0.000 5 | 0.007 6 | ^{163}Er | 0.000 3 | 0.007 2 |
| ^{156}Yb | 0.059 0 | 0.014 1 | ^{157}Yb | 0.062 0 | 0.013 8 |
| ^{158}Yb | 0.011 0 | 0.013 3 | ^{159}Yb | 0.013 5 | 0.013 0 |
| ^{160}Yb | 0.003 1 | 0.012 8 | ^{161}Yb | 0.003 7 | 0.012 1 |
| ^{162}Yb | 0.001 0 | 0.011 7 | ^{163}Yb | 0.001 1 | 0.011 3 |
| ^{164}Yb | 0.000 4 | 0.010 9 | ^{165}Yb | 0.000 4 | 0.010 5 |

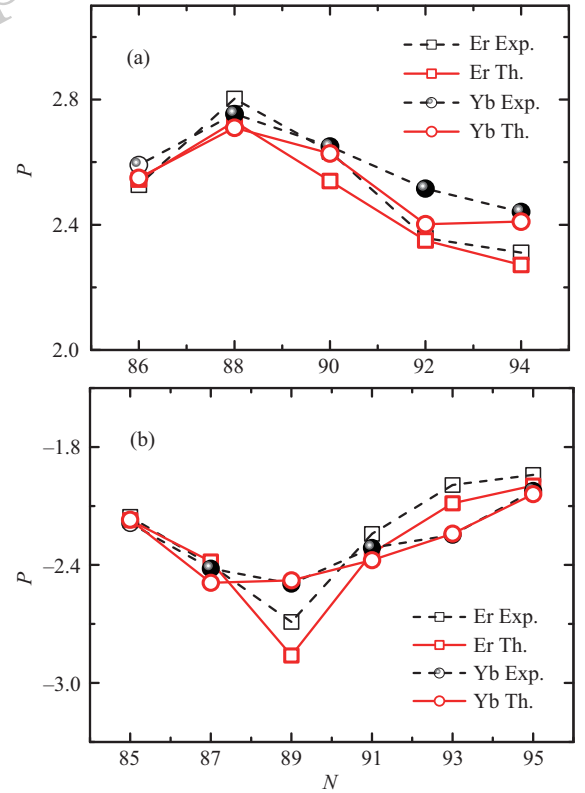


Fig. 3 (color online) The odd-even mass differences (in MeV) for $^{153-163}\text{Er}$ and $^{155-165}\text{Yb}$ as functions of neutron number N . Experimental values are denoted as “Exp.”, which are taken from Ref. [21], and the theoretical values calculated in the present model are denoted as “Th.” for (a) the even-even cases and (b) the odd- A cases.

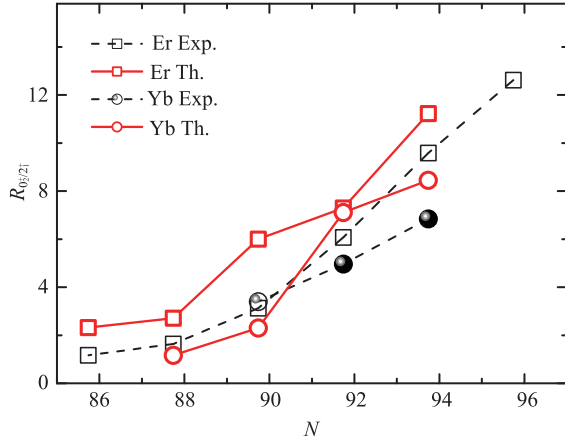


Fig. 4 (color online) The energy ratio of $^{154-164}\text{Er}$ and $^{156-164}\text{Yb}$ as functions of neutron number N . Experimental values are denoted as “Exp.”, which are taken from Ref. [21], and the theoretical values calculated in the present model are denoted as “Th.”.

for the even-even nuclei considered. For ^{154}Er ($N=86$) and ^{156}Er ($N=88$), the experimental and the theoretical value of the energy ratio are around $R_{0_2^+/2_1^+} \sim 3$ indicating a relatively stronger pairing interactions in this nucleus, while the experimental value of $R_{0_2^+/2_1^+}$ for ^{164}Er ($N=96$) is 13.69 corresponding to an axially deformed phase with weaker pairing interactions. Similarly, Yb isotopes exhibit the same pattern in Fig. 4. For ^{156}Yb ($N=86$) and ^{158}Yb ($N=88$), the theoretical value of the energy ratio is around $R_{0_2^+/2_1^+} \sim 3$ and both the experimental and the theoretical value of the energy ratio for ^{164}Yb ($N=94$) are around $R_{0_2^+/2_1^+} \sim 9$ which also over cross the strong pairing interactions phase, provide a sign of an axially deformed behavior. Those results confirm the analysis for Er and Yb isotopes in Fig. 3, the odd-even mass difference undergo the shape (phase) crossover from the spherical shape towards the axially deformed shape, in which the even-even nuclei with $N=88$ and odd-A nuclei with $N=89$ seem near to the critical point of the crossover. Furthermore, as shown in Fig. 5, I_H calculated from the present model indicate that the system undergoes the phase transition from the localized normal phase with $G^\nu=0$ and $I_H=0$ to the delocalized superconducting (pair condensate) phase with sufficiently large G^ν and $I_H \sim 1$ for $^{154-160}\text{Er}$. Particularly, the realistic G^ν value (red point in Fig. 5) crosses from the strong pairing interactions phase for ^{154}Er ($N=86$) to the localized normal phase for ^{160}Er ($N=92$). This result is also consistent to the critical region shown in Figs. 3~4. Thus, this work provides a microscopic picture of the ground-state shape (phase) crossover which may mainly be driven by the pairing interaction as revealed in the present model.

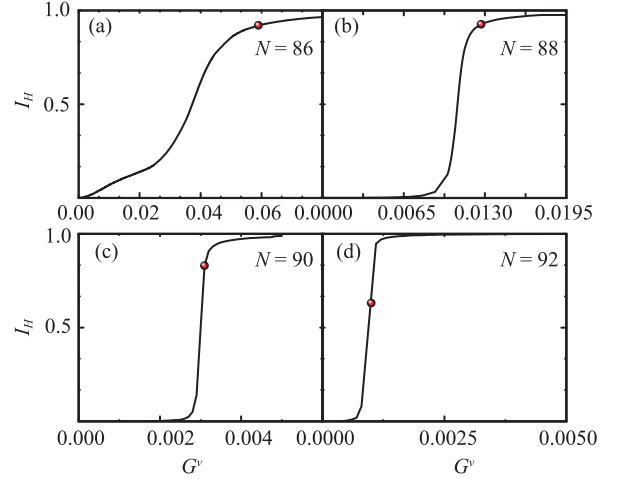


Fig. 5 (color online) The information entropy I_H (solid line) of the ground state as functions of G^ν (in MeV) for $^{154-160}\text{Er}$, the red point indicate the the corresponding G^ν value.

5 Conclusion

In summary, the Nilsson mean-field plus extended pairing model is applied to describe the ground-state shape (phase) crossover in Er and Yb isotopes. It is found that variation of the pairing interaction strength G and the deformation parameter ε_2 in the model alters the energy ratio $R_{0_2^+/2_1^+}$ and the ground-state occupation probabilities of valence nucleon pairs with different angular momenta. When G is small, the Nilsson mean-field is dominant, the system is in the axially deformed (rotational) shape (phase) with $R_{0_2^+/2_1^+} \sim 35$. With the increasing of G , $R_{0_2^+/2_1^+}$ changes non-monotonically for all the given ε_2 values considered. Particularly, a drastic change occurs around $G \sim 0.0078 \sim 0.012$ which marks the critical region of the crossover in the present model. Furthermore, when G is sufficiently large, the system is dominated by the pairing interaction with $R_{0_2^+/2_1^+} \sim 2$ corresponding to the spherical (vibrational) (shape) phase. This conclusion is consistent to that made in the $SU(3)$ - $U(5)$ transitional analysis within the interacting boson model (IBM) framework previously^[13]. It is observed that a critical region of the crossover exists as shown in the energy ratio $R_{0_2^+/2_1^+}$ for any value of the quadrupole deformation parameter, which is justified from the analysis of the ground-state information entropy of the model. Therefore, it seems that the shape (phase) crossover in the current model is mainly driven by the pairing interaction and less affected by the quadrupole deformation. As shown in our model fits to the energy ratio $R_{0_2^+/2_1^+}$ of $^{154-164}\text{Er}$ and $^{156-164}\text{Yb}$, the shape (phase) crossover indeed occurs in these isotopes, among which ^{156}Er and ^{158}Yb seem near to the critical point of the crossover. The en-

ergy ratio $R_{0_2^+/2_1^+}$ and the information entropy of the model all change noticeably within the critical region of the crossover.

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Er, Yb同位素链的基态形状(量子相)酷越研究

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摘要: 利用严格求解的Nilsson轴形变平均场加扩展对力模型, 对Er和Yb同位素链基态形状(量子相)酷越进行了研究。通过该模型下能级比 $R_{0_2^+/2_1^+}$ 、奇偶能差、信息熵的计算, 成功地再现了 $^{155-163}\text{Er}$ 和 $^{157-165}\text{Yb}$ 同位素相关物理量的形状(量子相)酷越行为。通过分析这些量随着四极形变参数和总体对力强度的变化过程, 显示了这种酷越行为主要是由于对力强度与四极形变之间的竞争导致的, 该结果揭示了本模型下的基态形状(量子相)酷越行为的来源。

关键词: 对力; 演化; 能级比

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