Shape phase transition in the odd Sm nuclei: effective order parameter and odd–even effect *

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Abstract: Some binding energy related quantities serving as effective order parameters have been used to analyze the shape phase transition in the odd Sm nuclei. It is found that the signals of phase transition in the odd Sm nuclei are greatly enhanced in contrast to the even Sm nuclei. A further analysis shows that the transitional behaviors related to pairing in the Sm nuclei can be well described by the mean field plus pairing interaction model, with a monotonic decrease in the pairing strength G.

Key words: shape phase transition, effective order parameter, odd–even effects

PACS: 21.60.Ev, 21.10.Re, 64.70.Tg **DOI:** 10.1088/1674-1137/39/10/104103

1 Introduction

Quantum phase transitions in nuclei have attracted a lot of attention from both experimental and theoretical perspectives [1–25], since they provide new insights into understanding the evolution of nuclear properties. The quantum phase transition is not of the usual thermodynamic type, but related to the equilibrium shape changes in the ground state of nuclei at zero temperature. It is thus also referred to as the shape phase transition or ground state phase transition, though the concept can also be applied to excited states. Evidence of the shape phase transition in nuclei is indicated experimentally through a sudden change in the properties of the ground state. An excellent example is provided by a set of even Sm isotopes, of which the evolution of its properties can be identified as the first-order shape phase phase transition experimentally [22]. On the other hand, odd-A nuclei can be approximately considered as systems with an even–even core coupled to a single valence nucleon. It is thus expected that the properties of odd-A nuclei should be definitely affected by the shape phase transition emerging along the related odd isotope or isotone chains.

Currently, analyses of the phase transitions in nuclei are mostly focused on even–even systems and have been carried out in the frame of phenomenological geometrical models of nuclear potential [1, 2], or algebraic models of nuclear structure [25] since the phase transitions in the intermediate and heavy mass region, such as the mass number $A\sim150$ region, are often out of reach of the microscopic shell models. In addition, phase transitions in odd-A nuclei may be more difficult to describe due to much more complicated dynamical situations [26] in contrast to the adjacent even–even species. However, if one only wants to emphasize some special aspects of nuclear phase transitions, the shell model (under some approximations) is still applicable to give a microscopic analysis of the phase transition in the $A\sim150$ region. The purpose of this work is to give a microscopic analysis of the shape phase transition in the odd Sm nuclei in terms of the effective order parameters and odd–even effects.

2 Effective order parameter

One way of addressing quantum phase transitions is to resort to the potential energy approach. To define phase transitions in theory, it is convenient to consider a schematic "Landau" potential [5] written as

$$V(\beta)=\beta^2+x[(1-\beta^2)^2-y\beta^3],\quad \beta\geqslant0, \tag{1}$$

with two control parameters $0\geqslant x\geqslant1$ and $y\geqslant0$. This kind of potential may be formally derived from the interacting boson model [25], which has been widely used to study quantum phase transitions in nuclei. It can be proven that the system has a second order phase transition at $x=x_{\rm c}=1/2$ when $y=0$ because the minima of

Received 14 January 2015
∗ Supported by National Natural Science Foundation of China (11375005, 11005056, 11175078, 11405080)
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$V(\beta)$, $V_{\rm min}$, and $\dfrac{\partial V_{\rm min}}{\partial x}$ are continuous, but $\dfrac{\partial^2 V_{\rm min}}{\partial x^2}$ is discontinuous. More generally, the system will show a first order phase transition as a function of x for any fixed value of $y>0$. For example, one can show that $V_{\rm min}$ is continuous but $\dfrac{\partial V_{\rm min}}{\partial x}$ is discontinuous at $x=x_{\rm c}=1/3$ when $y=2$, which indicates the first order phase transition occurring at $x_{\rm c}$. The potential (1) can be considered as a simplified phenomenological nuclear potential surface varying as the function of the deformation β, which indicates that one could take $\beta_{\rm equilib}=\beta_{\rm e}$ to be the order parameter. As shown for the cases considered in Fig. 1, the order parameter $\beta_{\rm e}$ changes continuously as a function of x, with the first derivative being discontinuous at $x_{\rm c}=1/2$ if $y=0$, corresponding to the second-order phase transition, while $\beta_{\rm e}$ jumps abruptly from 0 to 1 at

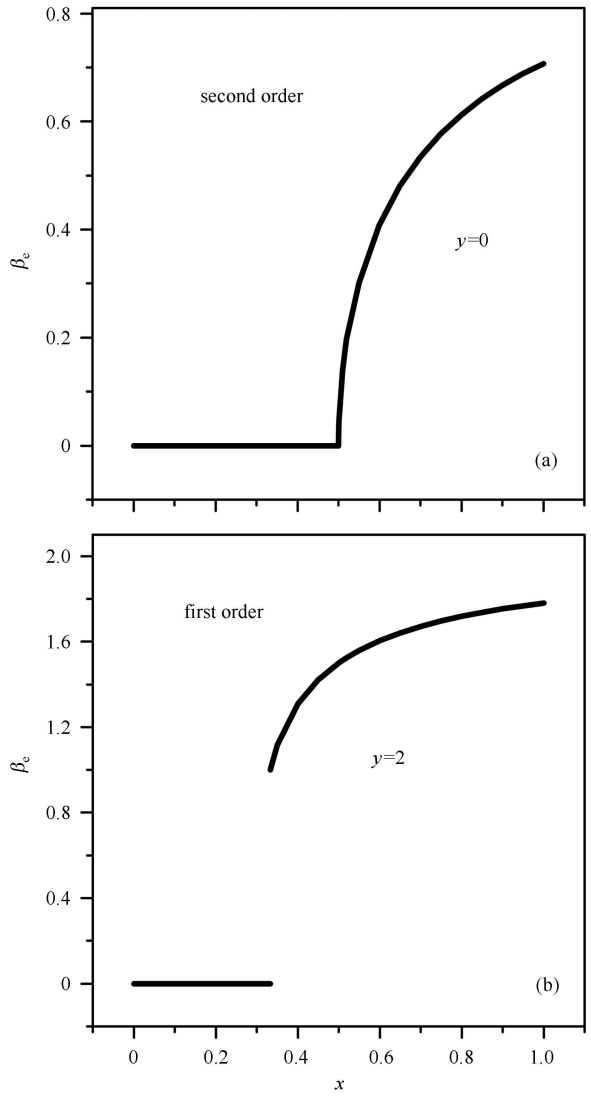

Fig. 1. The order parameter $\beta_{\rm e}$ as a function of x for $y=0$ and $y=2$, respectively.

$x_{\rm c}=1/3$ when $y=2$, corresponding to the first-order phase transition. It seems that both $\beta_{\rm e}$ and $V_{\rm min}$, which may correspond to the ground state deformation and energy respectively, can be used to identify the shape phase transition.

However, for real nuclei, things are considerably more complicated partly because $\beta_{\rm e}$ is not an observable. In fact, instead of $\beta_{\rm e}$, the so called effective order parameters [5] (observables sensitive to shape phase transitions occurring within nuclei) are often used to identify nuclear shape phase transitions and in some cases even determine their orders. The typical effective order parameters include the isomer shifts defined as $v=c[\langle r^2\rangle_{0_2}-\langle r^2\rangle_{0_1}]$ and $v'=c'[\langle r^2\rangle_{2_1}-\langle r^2\rangle_{0_1}]$ [5] with c and c' being the scale parameters, the B(E2) ratio $B({\rm E2};(L{+}2)_1\rightarrow L_1)/B({\rm E2};2_1\rightarrow 0_1)$ [16], and the energy ratio E_{L_1}/E_{0_2} [27], etc. Most of the effective order parameters are related to the quantum numbers of excited states, which makes it particularly difficult to use them to identify the phase transitions in odd nuclei. In contrast, the binding energy related quantities may serve as qualified effective order parameters to identify the phase transitions in both even–even and odd nuclei [17] since their values only depend on the number of nucleons, and their experimental data are also relatively abundant. On the other hand, the number of nucleons in nuclei is finite and the phase transitional behavior will be muted due to the finiteness of the system [5]. Specifically, instead of a discontinuity, sudden changes or flattening may be shown by the effective order parameters in nuclear shape phase transitions [5, 22].

3 Two-neutron separation energy

For an atomic nucleus, the most basic characteristic is nuclear mass or binding energy. The total binding energy $B(Z,N)$ for a nucleus with proton number Z and neutron number N is defined as [28]

$$B(Z,N)=ZM_{\rm p}+NM_{\rm n}-M(Z,N), \tag{2}$$

where $M_{\rm p}$ is the proton mass, $M_{\rm n}$ is the neutron mass, and $M(Z,N)$ denotes the nuclear mass. In experiments, data about the binding energy $B(Z,N)$ is also abundant in contrast to other observables. One may expect that the shape phase transition in an isotope should be reflected by the evolution of the binding energy, which for the Sm isotopes is shown in Fig. 2. However, the varied energy scale of the total binding energy $B(Z,N)$ in an isotope chain is too large ($\sim 10^2$ MeV) so that the signals of phase transition that are expected to appear around $N=90$ have been completely hidden behind the linear behavior of $B(Z,N)$ as shown in Fig. 2.

Thus one has to resort to other quantities related to the binding energy in order to identify the shape phase

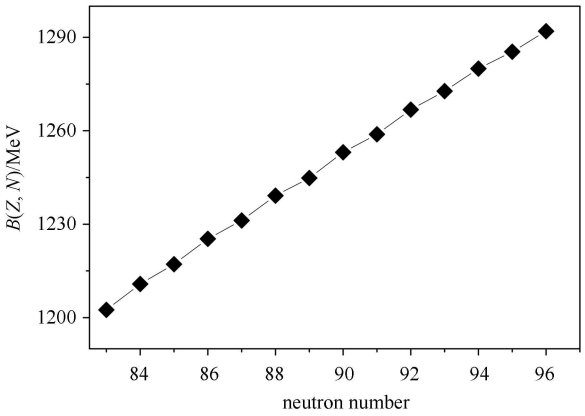

Fig. 2. Total binding energy $B(Z,N)$ for the Sm nuclei (taken from Ref. [29]) shown as functions of the neutron number.

transition in an isotope chain. For even–even nuclei, the two-neutron separation energy S_{2n}, which is defined as [28]

$$S_{2n}=B(Z,N)-B(Z,N-2), \quad (3)$$

can be considered as a primary and direct signature of the emergence of the shape phase transition [22, 24]. For odd-A nuclei, S_{2n} can also serve as a qualified effective order parameter for identifying the ground phase transitions [17]. For a set of isotopes, the two-neutron separation energy S_{2n} may be rewritten as a smooth contribution that is linear with the number of valence neutron pairs $N_{\rm p}$, plus a contribution from the deformation [26]

$$S_{2n}=-A-BN_{\rm p}+S(2n)_{\rm def}, \quad (4)$$

where A and B are the parameters. To emphasize the occurrence of the phase transition in the Sm nuclei, the experimental data of S_{2n} for both the even and odd Sm isotopes [17] are shown in Fig. 3, where the deformation contributions $S(2n)_{\rm def}$ are also shown to reveal the odd particle (single valence nucleus) effects on the phase transition.

It is easy to know from Eq. (4) that the deformation contributions $S(2n)_{\rm def}$ can be obtained from the data by subtracting a term linear with the number of valence neutron pairs $N_{\rm p}$. Specifically, the results of $S(2n)_{\rm def}$ are obtained from the data [29] fitted with $A=-19.8$ MeV and -19.4 MeV for the even and odd Sm nuclei respectively, and $B=0.66$ MeV according to (4). As clearly seen from Fig. 3(a), a noticeable feature is the sudden flattening near the neutron number $N=90$ shown by S_{2n} for the even Sm isotopes. Based on the analysis given in [22], the sudden flattening indicates the first order phase transition emerging in the corresponding isotopes. It is even more interesting to find that a similar or even more pronounced change appears in S_{2n} for the odd Sm isotopes near $N=90$, which indicates that the first-order phase transition also occurs in these odd Sm nuclei. As shown in Fig. 3(b), the phase transition occurring around $N=90$ corresponding to $N_{\rm p}=4$ is explicitly manifested in $S(2n)_{\rm def}$ for both the even and odd Sm isotopes. Thus $N_{\rm p}=4$ ($N=90$) may be considered as the critical point of the phase transitions in the Sm nuclei. Particularly, the phase transitional signal in the odd Sm nuclei seems to be greatly enhanced by the odd particle effect. Specifically, the amplitude of $S(2n)_{\rm def}$ in the odd Sm nuclei increases about 25% near the critical point in comparison to that in the even Sm nuclei.

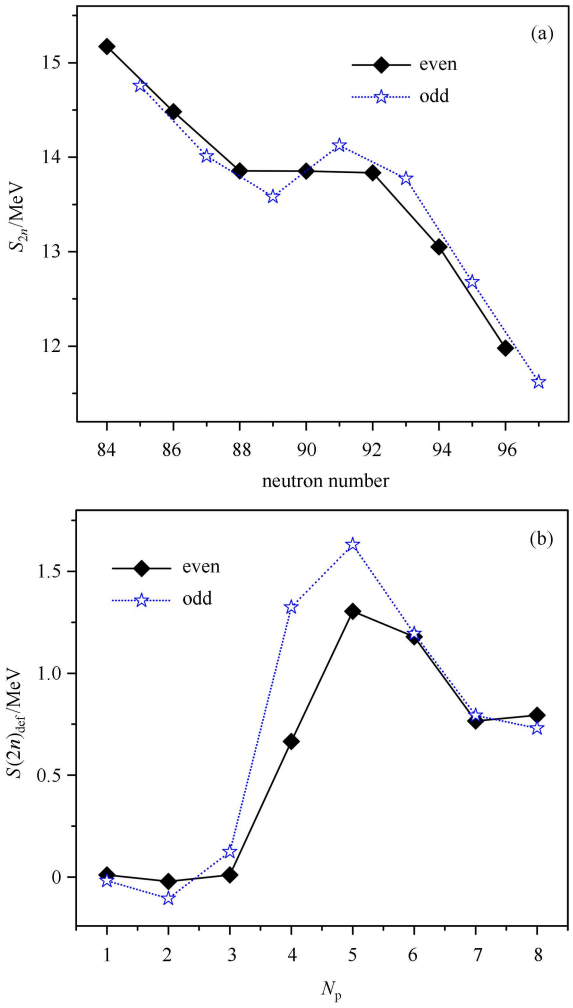

Fig. 3. (color online) The two-neutron separation energies, S_{2n} and their deformed part $S(2n)_{\rm def}$ for both the even and odd Sm nuclei are shown along the isotopes chain. The experimental data are taken from Ref. [29].

4 Odd–even mass difference and pairing excitation energy

Besides the two-neutron separation energy S_{2n} and its deformed part $S(2n)_{\rm def}$, there exist some other

binding-energy-related quantities that can serve as effective order parameters to identify the shape phase transitions in odd nuclei [17]. A novel transitional signal in odd–even nuclei related to the binding energy $B(Z,N)$ is given as the odd–even mass difference [17], which is defined as [28]

$$D=B(Z,N)-\frac{B(Z,N-1)+B(Z,N+1)}{2}. \quad (5)$$

Meanwhile, it is also well known that the odd–even effects, such as those in the odd–even mass difference, provide the most important evidence of pairing in nuclei [28]. Therefore, some microscopic factors relevant to pairing in manifesting the phase transition can be extracted from the odd–even effects. To do that, a shell model Hamiltonian including the deformed mean field and pairing interaction will be adopted to give a microscopic analysis of the phase transition related to pairing in the Sm nuclei. Specifically, the Hamiltonian is written as [28]

$$\hat{H}=\sum_i \epsilon_i\ (a_i^\dagger a_i+a_{\bar{i}}^\dagger a_{\bar{i}})+\sum_{i,j} G_{ij}\ b_i^\dagger b_j, \quad (6)$$

where ϵ_i represents the single-particle energy of the i-th Nilsson level, and $b_i^\dagger=a_i^\dagger a_{\bar{i}}^\dagger$ ($b_i=a_{\bar{i}}a_i$) is the pair creation (annihilation) operator with $\bar{i}$ labeling the time-reversed state of that labeled by i. To solve such a Hamiltonian, two approximation schemes are considered for the pairing interaction in this work. One is the nearest-orbit pairing-interaction model [30, 31], which is a simplified version of the Gaussian-type pairing interactions suitable for deformed nuclei [32] with the orbit-dependent pairing strengths written as

$$G_{ij}=\alpha\ \mathrm{e}^{-\beta(\epsilon_i-\epsilon_j)^2}, \quad (7)$$

where $\alpha<0$ and $\beta>0$ are the adjustable parameters. It is clear that the pairing strength G_{ij} shown in (7) is orbit-dependent, and the nearer the two orbits, the stronger the pairing interaction between the two pairs. As an approximation to the Gaussian-type interactions given in (7), only the on-orbit pairing interactions G_{ii} and the nearest-orbit pairing interactions G_{ii+1} or G_{ii-1} are considered in the nearest-orbit pairing model, while G_{ij} with $|i-j|\geqslant 2$ are ignored [30, 31]. As a further approximation, we set $G_{ii}=G_{ii\pm1}=G$. Thus, there is only one free-parameter G to be determined for each nucleus in the isotopes. Such a pairing interaction form can be exactly solved for all the Sm nuclei by directly diagonalizing the Hamiltonian in the valence nucleon space. More details about the solutions of the nearest-orbit pairing model can be found in Refs. [30, 31]. For convenience, we denote the exactly solvable nearest-orbit pairing interaction as the ENO scheme. Another approximation scheme is the constant pairing interaction [28], in which the paring strength is set as $G_{ij}=G$ for all the single-particle orbits i. However, the constant pairing interactions can be exactly solved only for a nucleus with very few valence nucleons, due to the difficulty of computation. To apply the constant pairing interactions form to the whole chain of the Sm isotopes, the well-known BCS method [28] is used to solve the corresponding Hamiltonian. We denote the constant pairing interaction solved by the BCS theory as the CBCS scheme.

By using the ENO and CBCS schemes, the odd–even mass difference D for the Sm nuclei has been fitted by the Nilsson mean-field plus the pairing model and the resulting values together with the experimental data are shown in Fig. 4. In theory, the odd–even mass difference is given as

$$D=-E_{\mathrm{g}}(Z,N)-\frac{-E_{\mathrm{g}}(Z,N-1)-E_{\mathrm{g}}(Z,N+1)}{2}, \quad (8)$$

where $E_{\mathrm{g}}(Z,N)$ is the ground state energy solved from

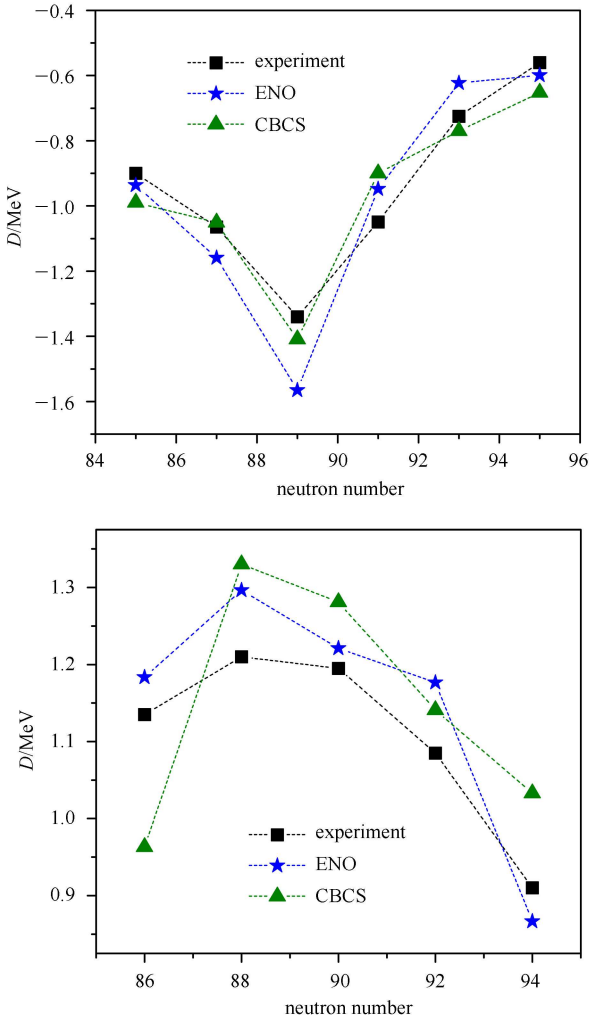

Fig. 4. (color online) (a) The odd–even mass difference D for Sm nuclei with neutron number $N=$ odd fitted by the pairing model in the two schemes; (b) the same as in (a) but for $N=$even.

(6) for a nucleus with the proton number Z and the neutron number N. In our calculations, the single-particle energies $\{\epsilon_i\}$ are calculated from the Nilsson model with deformation parameters taken from Ref. [33], which were determined systematically from the corresponding experimental data [34]. In addition, it is assumed that the odd–even mass difference in the Sm isotopes only comes from the neutron part since the proton number in a chain of isotopes is a constant. As is clearly seen from Fig. 4(a) and (b), the experimental values of the odd–even mass difference in Sm can be well reproduced in the pairing model for both schemes. Specifically, the values of the odd–even mass differences D are all negative for the odd Sm nuclei but positive for the even Sm nuclei, which indicates that even–even nuclei are more bounded than the odd–even nuclei [28]. More importantly, the evident phase transition signals in experiments shown by D, of which the values reach their minimum or maximum around $N=90$, are nicely expressed by those calculated from the pairing model. It is thus confirmed that the pairing interaction is indeed a key factor in driving phase transitions in nuclei.

Further, the fitted pairing strength G in the two schemes is shown in Fig. 5. As shown in Fig. 5(a) and (b), the resulting pairing strength G values in both schemes show a monotonic decrease for the even Sm isotopes as the neutron number N increases, except that the variational behavior of G in the ENO scheme is a little smoother than that in the CBCS scheme. A similar situation also appears in G for the odd Sm nuclei as seen in Fig. 5(c) and (d). It is thus confirmed that the phase transition behavior related to pairing in an isotope may be driven by the pairing interaction with a monotonic decrease in the pairing strength as the neutron number increases. In addition, one may find that the energy scale of G in the ENO scheme is almost ten times that in the CBCS scheme, as seen from Fig. 5. It is not difficult to understand this by considering the fact that only the on-orbit and nearest-orbits' pairing interaction are taken into account in the ENO scheme for a single-particle orbit i, in contrast to the CBCS scheme. It seems that the the transitional behavior of the odd–even mass differences D can be well illustrated in theory via the shell model Hamiltonian including only the mean-field plus pairing interaction.

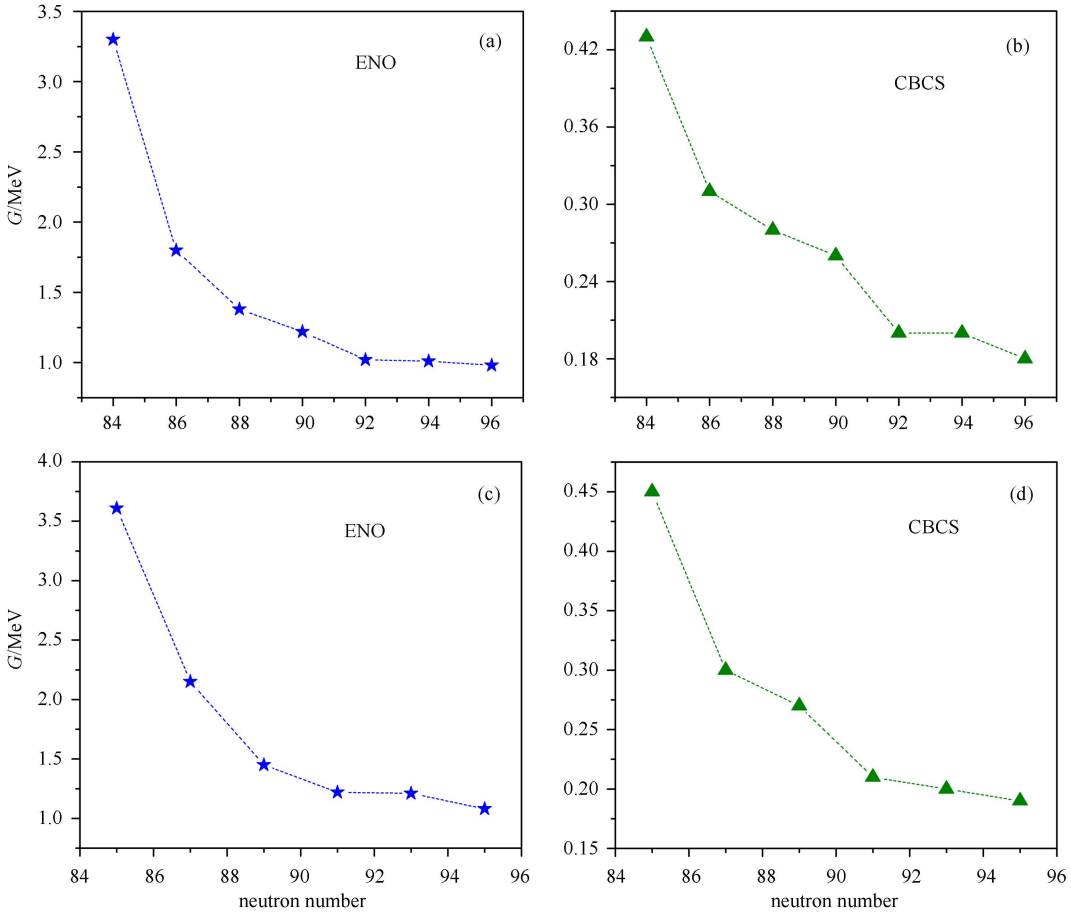

Fig. 5. (color online) The evolution of the pairing strength G changing as a function of neutron number.

To further reveal the phase transitional behaviors closely related to the pairing interaction, we also calculated the pairing-excitation energy (PEE) [31], which is also a quantity sensitive to the pairing strength G. Since the angular momentum projection along the third axis in the intrinsic frame is considered to be a conserved quantity in the model, the pairing-excitation states determined by the model are thus regarded approximately as excited states with the same spin and parity as those of the ground state of a nucleus. For example, the PEEs in the model for even–even nuclei are considered as the energies of the excited 0^+ state, $E_{0_n^+}$. In Fig. 6, the results of the first PEE calculated for the even Sm nuclei in the two schemes and the corresponding experimental data are shown. Notably, only the first neutron PEEs in the two schemes are taken to be compared with the experimental data since the proton PEE may be much higher than the corresponding neutron PEE in the present case. In the ENO scheme, the first PEE may be briefly denoted as $PEE = E_1 - E_g$, where E_1 and E_g represent the energy value of the first excited state and that of the ground state respectively, since broken pairs have not been taken into account in this scheme. In contrast, the first PEE calculated from the CBCS scheme can be explicitly given as

$$PEE = 2\sqrt{(\varepsilon_0 - \lambda)^2 + \Delta^2}, \tag{9}$$

where λ represents the Fermi energy, ε_0 denotes the single-particle energy closest to λ, and Δ is the so-called gap parameter [28]. All the parameters involved in (9) can be determined by the standard BCS theory [28]. As is clearly seen in Fig. 6, the first PEE in experiments also provides an evident phase transitional signal around $N = 90$. More importantly, such a phase transitional characteristic shown by the PEE can be well reproduced by the results calculated from the pairing model in the ENO scheme. It is thus further confirmed that the transitional characteristics in connection with pairing in the Sm isotopes are indeed driven by the pairing interaction with a monotonic decrease in the pairing strength. However, it can be also found that the PEE obtained from the constant pairing interactions in the CBCS scheme are much higher than those found experimentally, and the global behavior of the PEE in theory is also completely different from that in experiments. As a consequence, the exact solutions are important to explore the phase transition in the pairing model. It should be noted that the PEEs in the odd Sm nuclei are not taken into account here because some single-particle excitations with spin and parity the same as those of the ground state are often involved in the low-lying spectrum, which makes it difficult to pick out the PEE from the spectrum of the odd Sm nuclei.

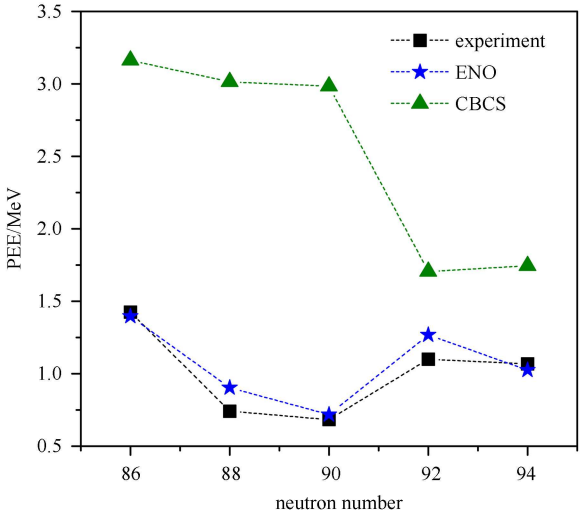

Fig. 6. (color online) The first pairing-excitation energy calculated by the two schemes compared with that determined by experiments [29].

5 Summary

In conclusion, we have made a microscopic analysis of the shape phase transition in the odd Sm nuclei from the point of view of the effective order parameter. Through analyzing the two-neutron separation energy, it is confirmed that the first order phase transition also occurs in the odd Sm isotopes as it does in the even Sm isotopes but with the signals of the phase transition in the odd species greatly enhanced by the odd neutron effect. It is also shown that the odd–even mass differences may reach their extreme value around the critical point, thus serving as a valid effective order parameter for the identification of the shape phase transition in the odd Sm nuclei. Particularly, analysis based on the mean-field plus pairing interaction Hamiltonian shows that the critical phenomena relevant to pairing in the Sm nuclei can be driven by the pairing interaction with a monotonic decrease in the pairing strength G. In addition, the results also indicate that the exactly solvable models are important to analyze transition characteristics related to pairing in the excited states. Although the discussion in this work provides a specific example of microscopic analysis of the shape phase transition in odd-A nuclei, investigations based on a more realistic shell model Hamiltonian with different truncation schemes [6, 35, 36] are still needed to eventually confirm or disprove the theoretical predictions.

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