Nucleon-pair approximations for low-lying states of even-even $N = Z$ nuclei

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In this paper we study nucleon-pair correlations of low-lying states for two typical cases of even-even $N = Z$ nuclei. The first case is a single $g_{9/2}$ shell with eight valence nucleons. In this case we study S-pair, isoscalar spin-aligned-pair, isoscalar spin-one-pair approximations, with both schematic and realistic interactions. We find that electric quadrupole transition rates and electric quadrupole moments exhibit different patterns depending on the pair-truncated scheme. In the second case we study ground states of ^{20}Ne, ^{24}Mg, ^{32}S, ^{36}Ar, ^{44}Ti, ^{48}Cr, ^{60}Zn, ^{64}Ge, ^{92}Pd, and ^{96}Cd. For ground states of these nuclei, the S-pair approximation is reasonably good (though not as good as for semimagic nuclei); the isoscalar spin-one-pair approximation is not very good. The isoscalar spin-aligned pair approximation is good for ground states of ^{44}Ti and ^{96}Cd, and not very good for ^{48}Cr and ^{92}Pd. The effect of the spin-orbit coupling strength on pairing correlations is studied. Our calculations suggests that the spin-orbit coupling favors the S-pair correlation in ground states of $N = Z$ nuclei.

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I. INTRODUCTION

The pairing correlation plays an important role in nuclear structure. Nucleon pairs with spin $J = 0$ (denoted by S pairs) are dominant ingredients in low-lying states of semimagic nuclei [1], as a consequence of the strong monopole pairing interaction between like nucleons. Such isovector pairing correlation has been emphasized in the seniority scheme [2], the BCS theory [3–6], the interacting boson model [7], the broken pair model [8,9], and the nucleon-pair approximation of the shell model [10]. See Ref. [11] for a comprehensive review.

In addition to isovector pairing interaction, isoscalar pairing interaction is strong. This can be seen from the δ interaction for two nucleons in a single-j orbit: spin $J = J_{\max} = 2j$ and $J = 1$ states achieve very low energies. Therefore the isoscalar spin-aligned $J = J_{\max}$ pair approximation and isoscalar deuton-like $J = 1$ pair (namely the P pair) approximation might provide us with proper scenario for low-lying states of nuclei with equal numbers of protons and neutrons [12].

Indeed, studies of the isoscalar spin-aligned pair could be traced back to the so-called stretch scheme in 1966 [13], and particularly in recent years the spin-aligned pairs of the $g_{9/2}$ orbit were suggested to be dominant building blocks in low-lying states of a few $N = Z$ nuclei below the doubly magic nucleus, ^{100}Sn [14–25]. On the other hand, it was also pointed out that the spin-aligned pair approximation is not the unique scenario for these cases; for instance, Refs. [14,26] showed that the seniority scheme is also relevant in the ground state of two valence protons and two valence neutrons, and of four valence protons and four valence neutrons; Refs. [19,27] showed that both isovector pairs and isoscalar pairs can provide good descriptions in low-lying states of ^{20}Ne, ^{24}Mg, ^{92}Pd, and ^{96}Cd. Such dual description is a consequence of the nonorthogonality of nucleon-pair basis. Analytical formulas of the overlap between wave functions with the lowest seniority quantum number and the spin-aligned pair approximation for $T = 0$ states of four nucleons are given in Ref. [27].

The isoscalar P-pair correlation has also attracted considerable attention. A number of approaches, such as the exactly solvable SO(5) and SO(8) models of isoscalar and isovector pairing, the mean field approaches, and the nuclear shell model studies with the "pair counting" operators, have been applied to study P-pair correlation in low-lying states of $N \approx Z$ nuclei. A summary of isoscalar pairing correlation was recently given in Ref. [28].

The purpose of this paper is to study isovector and isoscalar pair approximations for low-lying states of even-even $N = Z$ nuclei, in terms of the nucleon-pair approximation of the shell model [10,11,29]. We calculate level energies, wave functions, electric quadrupole transition rates, as well as electric-quadrupole moments in nucleon-pair bases. This paper is organized as follows. In Sec. II we study eight valence nucleons in a single $j = 9/2$ shell, with both schematic and effective interactions. In Sec. III we study pair correlations in the ground states of $N = Z$ even-even nuclei, including ^{20}Ne, ^{24}Mg, ^{32}S, ^{36}Ar, ^{44}Ti, ^{48}Cr, ^{60}Zn, ^{64}Ge, ^{92}Pd, and ^{96}Cd. In Sec. IV we summarize our results.

II. SINGLE-j SHELL CALCULATION

The ground states of two protons and two neutrons, and of four valence protons and four valence neutrons in a single-j shell were studied by Neergård in Refs. [14,26], in terms of both the seniority scheme and the spin-aligned isoscalar pair approximation. In Ref. [27] the seniority scheme, the spin-aligned pair approximation, and the P pair approximation were applied to low-lying states with spin $0,2,\ldots,8$ and isospin 0, of four nucleons in a single-j shell. In this section we study nucleon-pair approximations for low-lying states of eight

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nucleons in a single $j = 9/2$ shell, for both schematic and realistic interactions.

We use I and T to denote the total spin and isospin of a given state, respectively; we use J and M to denote the spin of one nucleon pair and its z-component projection, respectively; we use $\mathbb{T}$ and τ to denote the isospin of one nucleon pair and its z-component projection, respectively. For a single-j shell, $\mathbb{T} = 1$ if J is even, and $\mathbb{T} = 0$ if J is odd. For simplicity the index $\mathbb{T}$ is suppressed without confusion.

The simplest schematic interaction is the zero-range δ interaction (denoted by V_δ), and the two-body matrix elements $\langle j^2 J|V_\delta|j^2 J\rangle$ are the lowest in energy for $J = 0$ (with $\mathbb{T} = 1$), $J = 1$ or $2j$ (with $\mathbb{T} = 0$) in the case of a single-j shell. Therefore we assume our schematic interaction as follows:

$$H(a,b) = (1 - a - b)V_{J=0} + aV_{J=2j} + bV_{J=1}, \qquad (1)$$

where a and b are adjustable parameters ranging between 0 to 1, and

$$V_J = -\sum_{M=-J}^{J}\sum_{\tau=-\mathbb{T}}^{\mathbb{T}} A_{M\tau}^{(J\mathbb{T})^\dagger} A_{M\tau}^{(J\mathbb{T})},$$
$$A_{M\tau}^{(J\mathbb{T})^\dagger} = \frac{1}{\sqrt{2}}(a_j{}^\dagger \times a_j{}^\dagger)_{M\tau}^{(J\mathbb{T})},$$

where $a_j{}^\dagger$ is the creation operator of a nucleon in the j orbit.

A. Framework

In the nucleon-pair approximation [11], the building blocks of a wave function are nucleon pairs with given spin and isospin. For $2N$ valence nucleons, N nucleon pairs are coupled successively, i.e.,

$$A^{(J_N)^\dagger}(r_1 \cdots r_N, J_1 \cdots J_N) \equiv \left(\cdots\left(\left(A^{(r_1)^\dagger} \times A^{(r_2)^\dagger}\right)^{(J_2)} \times A^{(r_3)^\dagger}\right)^{(J_3)} \times \cdots \times A^{(r_N)^\dagger}\right)^{(J_N)}, \qquad (2)$$

where $A^{(r_i)^\dagger} = (a_j{}^\dagger \times a_j{}^\dagger)^{(r_i)}$ denotes a nucleon pair with spin J_{r_i} and isospin $\mathbb{T}_{r_i}$; (r_i) is short for $(J_{r_i}, \mathbb{T}_{r_i})$; (J_i) is short for (J_i, T_i).

In the quasispin formalism with isospin [30,31], the wave function of eight nucleons with the lowest seniority number of $I = 0,2,\ldots,8$ and $T = 0$ is written as

$$|\Psi_{\rm LS}(I)\rangle = \left(\left((S^\dagger \times S^\dagger)^{(0,0)} \times S^\dagger\right)^{(0,1)} \times A^{(I,1)^\dagger}\right)^{(I,0)}|0\rangle, \qquad (3)$$

where we use the subscript "LS" to represent the abbreviation "lowest seniority", and $S^\dagger = A^{(0,1)^\dagger}$. This wave function is not normalized. We note that in the notation of Flowers [32] the above "LS" wave function has $(s,t) = (0,0)$ for $I = 0$ and $(s,t) = (2,1)$ for $I = 2,4,6,8$, where s is the seniority number and t is the reduced isospin. It is also noted that Eq. (3) is very similar to the pair basis used in the broken pair approximation [8,9].

In the spin-aligned pair approximation, the basis states are constructed by four isoscalar pairs with $J = 9$,

$$|\Psi_{\rm SA}\rangle = \left(\left((A^{(9,0)^\dagger} \times A^{(9,0)^\dagger})^{(J_2,0)} \times A^{(9,0)^\dagger}\right)^{(J_3,0)} \times A^{(9,0)^\dagger}\right)^{(I,0)}|0\rangle, \qquad (4)$$

where J_2 and J_3 are intermediate spins. By choosing intermediate spins in all possible ways, one gets a set of states that are generally linearly dependent. From this set we select a maximal linearly independent subset, which is determined by inspection of the norm matrix, that is, the matrix of inner products, by using as the criterion for linear independence that it has only nonzero eigenvalues. The subset can be chosen in several equivalent ways. The calculated states are then obtained by diagonalization of Hamiltonian matrix in the space spanned by the selected subset of states. The maximum spin I of a state $|\Psi_{\rm SA}\rangle$ is 24, and the numbers of states with even I (=0,2,4, ...,24) are 3,4,6,7,7,7,7,5,4,3,2,1,1, respectively. The subscript "SA" refers to the abbreviation of "spin aligned".

In the P-pair approximation, we take two configurations. The first is the P-pair condensation, i.e.,

$$|\Psi_{\rm SO1}\rangle = \left(\left((P^\dagger \times P^\dagger)^{(J_2,0)} \times P^\dagger\right)^{(J_3,0)} \times P^\dagger\right)^{(I,0)}|0\rangle, \qquad (5)$$

where $P^\dagger = A^{(1,0)^\dagger}$. The maximum spin I of a state $|\Psi_{\rm SO1}\rangle$ is 4. The state with even values of I is unique, and states with odd values of I do not exist. Thus the intermediate spin J_2 is equal to either 0 or 2, and J_3 is equal to either 1 or 3. The number of states and the intermediate spins for the P-pair condensation system are exactly the same as those for a spin-one boson (i.e., p boson) system. For a system with n spin-one bosons, the number of state is 1 for even values of $I + n$, and is 0 for odd values of $I + n$. This fact can be proved straightforwardly via the m-scheme method [33]. Therefore the above basis is the wave function of H in the P-pair condensation subspace. The subscript "SO" refers to the abbreviation "spin one". The second configuration is constructed by three P pairs and one isoscalar pair, i.e.,

$$|\Psi_{\rm SO2}\rangle = \left(\left((P^\dagger \times P^\dagger)^{(J_2,0)} \times P^\dagger\right)^{(J_3,0)} \times A^{(J,0)^\dagger}\right)^{(I,0)}|0\rangle, \qquad (6)$$

where J_2 and J_3 are intermediate spins, and J is the spin of the fourth pair which is equal to 1,3,5,7, or 9. The basis states are chosen in the same way as they are in the SA space. The maximum spin I of a state $|\Psi_{\rm SO2}\rangle$ is 12, and the numbers of states with I (=0,2,4, ...,12) are 2,4,6,6,5,3,1, respectively. Finally, we denote the calculated wave functions in the full shell model space by $|\Psi_{\rm SM}\rangle$, where "SM" stands for "shell model".

B. Pair approximation with schematic interactions

In this paper we call the quantity $\langle\Psi_a|\Psi_b\rangle^2$ the overlap between two states, $|\Psi_a\rangle$ and $|\Psi_b\rangle$. We calculate overlaps of the pair-truncated wave functions $|\Psi_{\rm LS}\rangle, |\Psi_{\rm SA}\rangle, |\Psi_{\rm SO1}\rangle, |\Psi_{\rm SO2}\rangle$ with shell model wave functions $|\Psi_{\rm SM}\rangle$, for low-lying states of eight nucleons with $I = 0,2,\ldots,8$ and $T = 0$ in the single $j = 9/2$ shell. We also calculate the reduced electric-quadrupole transition probability $[B(E2)]$ between these states and the

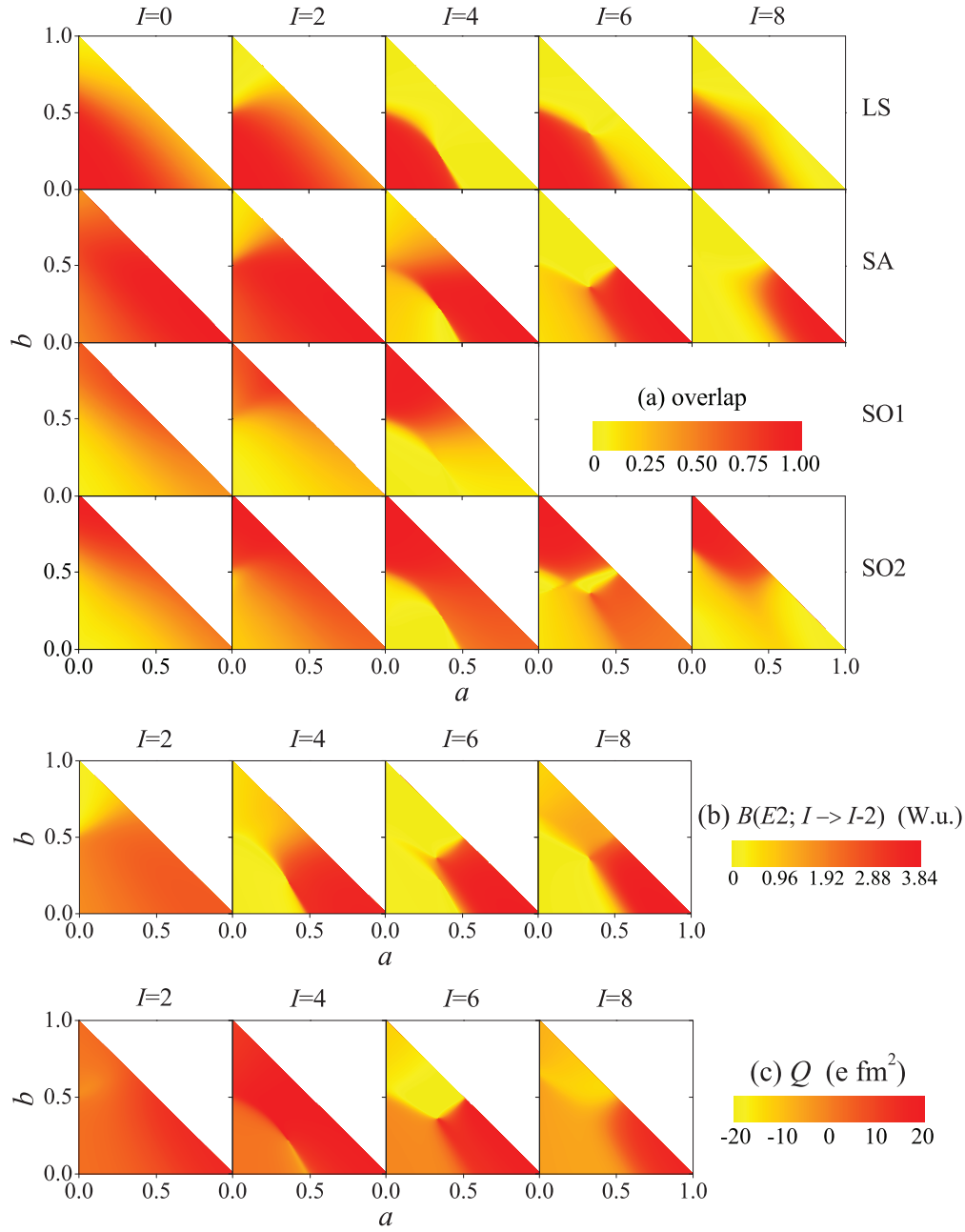

FIG. 1. (Color online) Nucleon-pair approximation for yrast $T = 0$ states with spin $I = 0,2,4,6,8$, for eight nucleons in the single $j = 9/2$ shell with schematic Hamiltonian $H(a,b) = (1 - a - b)V_{J=0} + aV_{J=2j} + bV_{J=1}$, where a and b are adjustable parameters between 0 to 1. (a) Overlaps between pair-truncated wave functions and the shell model wave functions. (b) $E2$ transition rates between yrast $T = 0$ states. (c) electric quadrupole moments of yrast $T = 0$ states. The abbreviations "LS", "SA", "SO1", and "SO2" represent the lowest seniority scheme [see Eq. (3)], the isoscalar spin-aligned pair approximation [see Eq. (4)], the P pair condensation [see Eq. (5)], and the subspace constructed by three P pairs plus another isoscalar pair [see Eq. (6)], respectively.

electric-quadrupole moment (Q), by using the shell model wave functions. The effective charges are simply taken to be 1 for valence protons and 0 for valence neutrons. Because the relative values of $B(E2)$ and Q are independent of the effective charges for $N = Z$ nuclei, the general feature of $B(E2)$ and Q does not depend on specific values of effective charges.

The calculated results are shown in Fig. 1. The transverse axis and the vertical axis in Fig. 1 correspond to the adjustable parameters a and b, respectively, in the Hamiltonian of Eq. (1). The first, second, third, fourth, and fifth columns in Fig. 1(a) correspond to states with $I = 0,2,\ldots,8$, respectively. Overlaps of $|\Psi_{\rm LS}\rangle$, $|\Psi_{\rm SA}\rangle$, $|\Psi_{\rm SO1}\rangle$, $|\Psi_{\rm SO2}\rangle$ with $|\Psi_{\rm SM}\rangle$ are presented in each of the four rows. One sees that the yrast $I = 0$–8 states are very well described by the seniority scheme in the cases with a strong $J = 0$ pairing interaction (where both a and b are small), and are very well described by the spin-aligned pair approximation if the $J = 2j$ pairing interaction is strong (where a is close to 1). On the other

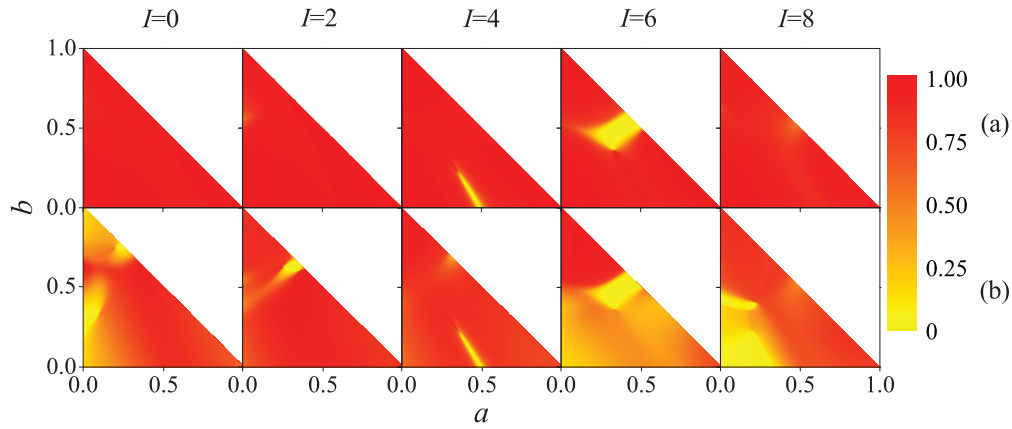

FIG. 2. (Color online) Overlaps between wave functions of the "LS+SA+SO2" pair subspace and those of the shell model space. (a) Yrast $T = 0$ states, and (b) the second lowest spin I states with $T = 0$. Abbreviations "LS", "SA", and "SO2" are the same as in Fig. 1.

hand, in the limit of strong $J = 1$ pairing interaction (b is close to 1), $\langle\Psi_{\rm SO1}(I)|\Psi_{\rm SM}(I_1^+)\rangle^2$ is about 0.62 and 0.66 for the yrast $I = 0$ and 2 states, respectively, and is close to 1 for the yrast $I = 4$ state; the P pair condensation is not a very good approximation for the yrast $I = 0,2$ states and very good for the yrast $I = 4$ state. Interestingly, all yrast even $I =$ 0-8 states are very well described by $|\Psi_{\rm SO2}\rangle$ in the limit of strong $J = 1$ pairing interaction.

In Ref. [27] the analytical formula of the overlap between the wave function with the lowest seniority number and the spin-aligned pair-truncated wave function is given for $T = 0$ states with $I = 0,2,\ldots,2j-1$ of four nucleons in a single-j shell. One can use the formula to calculate the overlap, which is close to 0 for $I \sim 2j-1$, and relatively large for $I \approx 2$. For eight nucleons, it is impossible to derive the analytical formula of $\langle\Psi_{\rm LS}|\Psi_{\rm SA}\rangle^2$. Yet numerical calculations show the similar pattern. In the limit of large a and small b (where the spin-aligned pair approximation is good), the value of $\langle\Psi_{\rm LS}(I)|\Psi_{\rm SM}(I_1^+)\rangle^2$ is smaller than 0.1 for $I \geqslant 4$, and is equal to ∼0.4 for $I = 2$ and ∼0.3 for $I = 0$. For small a and b [where the seniority scheme is good, see the second row of Fig. 1(a)], $\langle\Psi_{\rm SA}(I)|\Psi_{\rm SM}(I_1^+)\rangle^2$ is close to 0 for $I \geqslant 4$, and ∼0.6 for $I = 2$ and ∼0.5 for $I = 0$. In the cases with small a and large b (where $|\Psi_{\rm SO2}\rangle$ is good), $\langle\Psi_{\rm LS}(I)|\Psi_{\rm SM}(I_1^+)\rangle^2$ is smaller than 0.1, and $\langle\Psi_{\rm SA}(I)|\Psi_{\rm SM}(I_1^+)\rangle^2$ is ∼0.4 for $I = 0$, and smaller than 0.01 for $I =$ 2,4,6, and 8.

The behaviors of the $E2$ transition rates and the electric-quadrupole moments are very interesting. In Fig. 1(b) our calculated $E2$ transition rates are presented in the Weisskopf unit. In the case of strong $J = 0$ pairing interaction, the $E2$ transition rates of $4_1^+ \to 2_1^+, 6_1^+ \to 4_1^+$, and $8_1^+ \to 6_1^+$ are close to 0. In the case of strong $J = 2j$ pairing interaction, the relative $E2$ transition rates of $4_1^+ \to 2_1^+, 6_1^+ \to 4_1^+$, and $8_1^+ \to 6_1^+$ with respect to $2_1^+ \to 0_1^+$ are all approximately equal to 1.5. In the case with a strong $J = 1$ pairing interaction, the relative $E2$ transition rates exhibit a staggering behavior [$B(E2)$ of $4_1^+ \to 2_1^+, 6_1^+ \to 4_1^+$, and $8_1^+ \to 6_1^+$ with respect to $2_1^+ \to 0_1^+$ are approximately equal to 2.6, 0.2, and 3.4, respectively].

The electric-quadrupole moment for the yrast $T = 0$ states of eight nucleons is presented in Fig. 1(c). In the large a limit, Q for $I =$ 2, 4, 6, 8 is positive and larger than 15 $e$fm^2; in the large b limit, the value of Q is larger than 11 $e$fm^2 for $I = 4$ and smaller than -12 $e$fm^2 for $I = 6$; and in the limit of small a and b, Q is very small. It is noted that for eight-nucleon holes in the $j = 9/2$ shell (such as ^{92}Pd), the values of Q in Fig. 1(c) should be multiplied by -1 due to the particle-hole transformation. The very different behaviors of $B(E2)$ and Q mentioned above might be useful to predict which pair approximation is important in the $T = 0$ states of eight nucleons in a single-j shell.

We investigate the validity of the "LS+SA+SO2" pair approximation, in which the "LS", "SA", and "SO2" subspaces are all included in the configuration. We calculate overlaps between the wave functions of the "LS+SA+SO2" space and those of the shell model space for the yrast and the second lowest states of $I = 0,2,\ldots,8$ and $T = 0$, and present the values in Fig. 2. One sees that the overlaps are mostly close to 1 in the yrast states. However, the overlap evolves quickly in a few specific regions. For example, for $a \approx 0.4$ and $b \approx 0.5$ in row (a) of Fig. 2, the value of overlap for the $I = 6$ state becomes unexpectedly small. In the second lowest states, the overlap changes irregularly.

C. Pair approximation with realistic interactions

Now we come to the nucleon-pair approximation with realistic interactions. As in the case of schematic interactions, here we calculate overlaps between wave functions obtained in a few pair-truncated spaces and those obtained in the exact shell model space, for the yrast states with $I = 0,2,\ldots,8$ and $T = 0$ of eight nucleons in the single-$1g_{9/2}$ shell but with realistic interactions. Many realistic interactions were obtained for the single-$1g_{9/2}$ shell, and we adopt ten sets of them [15,16,34–38], denoted by (a)–(j), respectively, in the same sequence as in Ref. [27] (see Table I therein).

Reference [26] showed that the 0_1^+ state for a nucleus with four valence protons and four valence neutrons is composed of 75% of the seniority-zero wave function (the S pair condensation) with $(s,t) = (0,0)$. In Fig. 3, we obtain similar results for the 0_1^+ state. The lowest seniority wave function is reasonably good for the 0_1^+ and 2_1^+ states, and becomes almost irrelevant for the 4_1^+ and 6_1^+ states. For the 8_1^+ state, $\langle\Psi_{\rm LS}|\Psi_{\rm SM}\rangle^2$

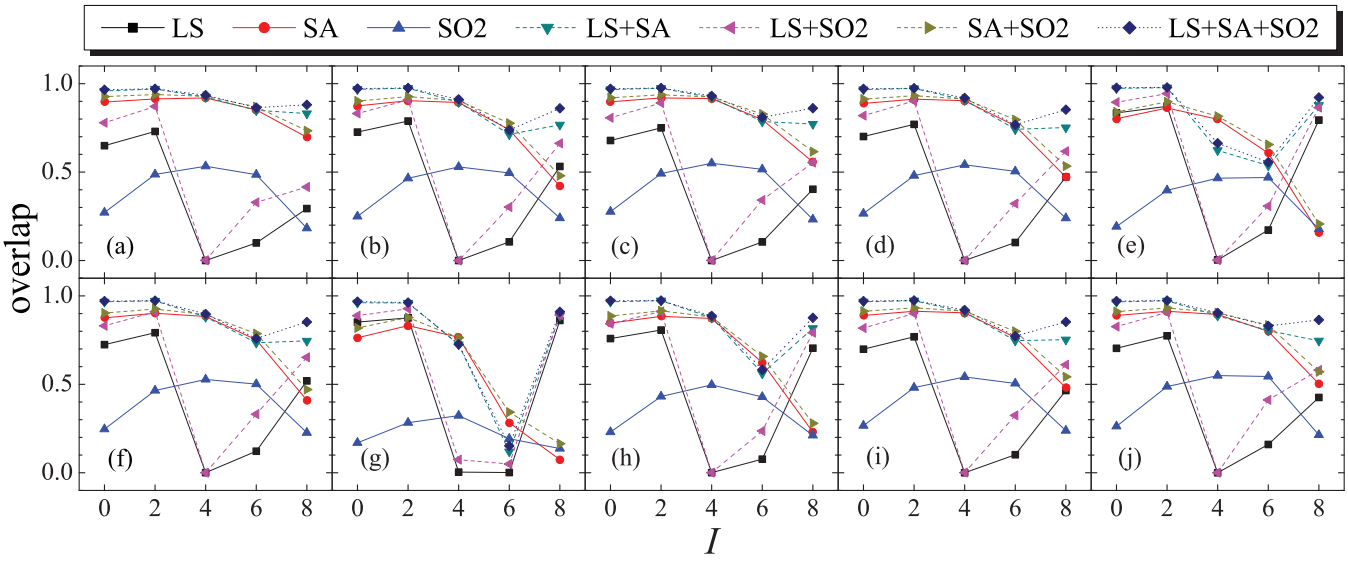

FIG. 3. (Color online) Overlaps between wave functions of pair-truncated spaces and those of the shell model space for the lowest $I = 0,2,\ldots,8$ and $T = 0$ states of eight nucleons in a single $j = 9/2$ shell, by using effective interactions (a)–(j). The abbreviations "LS", "SA", and "SO2" are the same as in Fig. 1.

is sensitive to the specific interaction, and its value ranges from 0.29 to 0.86 for the effective interactions (a)–(j). We also note here that although the overlap $\langle\Psi_{\rm LS}|\Psi_{\rm SM}\rangle^2$ is large for the yrast $I = 0,2$ states, the energies of $|\Psi_{\rm LS}\rangle$ are very different from the shell model results, see Fig. 4.

In the single $g_{9/2}$ shell calculations, low-lying states of a nucleus with four valence protons and four valence neutrons have been found to be well represented by the spin-aligned pair approximation [15,17,24–26], and for the ground state the spin-aligned pair approximation provides us with a more proper picture than the S pair approximation [17,26]. In Fig. 3, one sees that this is indeed the case: for the 0_1^+, 2_1^+ and 4_1^+ states, the spin-aligned pair approximation remarkably well reproduces the shell model results of the $g_{9/2}$ shell. For the 8_1^+ state, $\langle\Psi_{\rm SA}|\Psi_{\rm SM}\rangle^2$ depend on the interactions. The P pair approximation is not good for any of these yrast states.

One might be interested in the calculated results in the space spanned by our above pair-truncated subspaces, which include the "LS+SO2", "SA+SO2", "LS+SA", and "LS+SA+SO2" spaces. The "LS+SO2" space is the space spanned by $\Psi_{\rm LS}$ and $\Psi_{\rm SO2}$; the "SA+SO2" space is the space spanned by $\Psi_{\rm SA}$ and $\Psi_{\rm SO2}$; the "LS+SA" space is the space spanned by $\Psi_{\rm LS}$ and $\Psi_{\rm SA}$. We present the overlaps between the wave functions in these configurations and the SM results in Fig. 3. One sees that the "LS+SO2" subspace does not substantially improve the overlaps in comparison with the overlaps of the "LS" subspace; nor the "SA+SO2" subspace substantially improves the overlaps in comparison with the overlaps of the "SA" subspace. The "LS+SA" and "LS+SA+SO2" spaces are remarkably good for all the states, except for the case with the interaction (g).

Finally, we present energy spectra calculated in the "SM", "LS", "SA", and "SO2" spaces with the realistic interaction (a). In Fig. 4, the spin-aligned pair approximation well reproduces spectra obtained in the "SM" space. The spin-aligned pair approximation shows an underbinding of ∼0.5 MeV for the ground state, and this underbinding shrinks to ∼0.2 MeV if the contribution of S pairs is taken into account. This result is consistent with the result in Refs. [15,25]. Neither the lowest seniority scheme nor the P pair approximation reproduces the spectra well.

III. NUCLEON-PAIR CONDENSATION IN REALISTIC NUCLEI

To proceed our discussion, we define the shell model Hamiltonian for many-j shells,

$$H_{\rm eff} = H_0 + V_{\mathbb{T}=1} + V_{\mathbb{T}=0}. \tag{7}$$

Here the first term, H_0, is the single-particle energy term,

$$H_0 = \sum_j \epsilon_{nlj} \sum_{m\tau} a_{jm\tau}{}^\dagger a_{jm\tau}, \tag{8}$$

where ϵ_{nlj} is the single-particle energy of orbit with quantum numbers n,l,j. The second and third terms in Eq. (7), $V_{\mathbb{T}=0}$ and $V_{\mathbb{T}=1}$, are the isoscalar and isovector two-body interactions, respectively,

$$V_{\mathbb{T}=0} = \sum_J \sum_{j_1\leqslant j_2} \sum_{j_3\leqslant j_4} \frac{V_{J0}(j_1j_2j_3j_4)}{\sqrt{(1+\delta_{j_1j_2})(1+\delta_{j_3j_4})}} \times \sum_m A^{(J0)}_{m0}(j_1j_2)^\dagger A^{(J0)}_{m0}(j_3j_4),$$

$$V_{\mathbb{T}=1} = \sum_J \sum_{j_1\leqslant j_2} \sum_{j_3\leqslant j_4} \frac{V_{J1}(j_1j_2j_3j_4)}{\sqrt{(1+\delta_{j_1j_2})(1+\delta_{j_3j_4})}} \times \sum_{m\tau} A^{(J1)}_{m\tau}(j_1j_2)^\dagger A^{(J1)}_{m\tau}(j_3j_4),$$

where V_{J0} and V_{J1} are isoscalar and isovector two-body matrix elements, respectively.

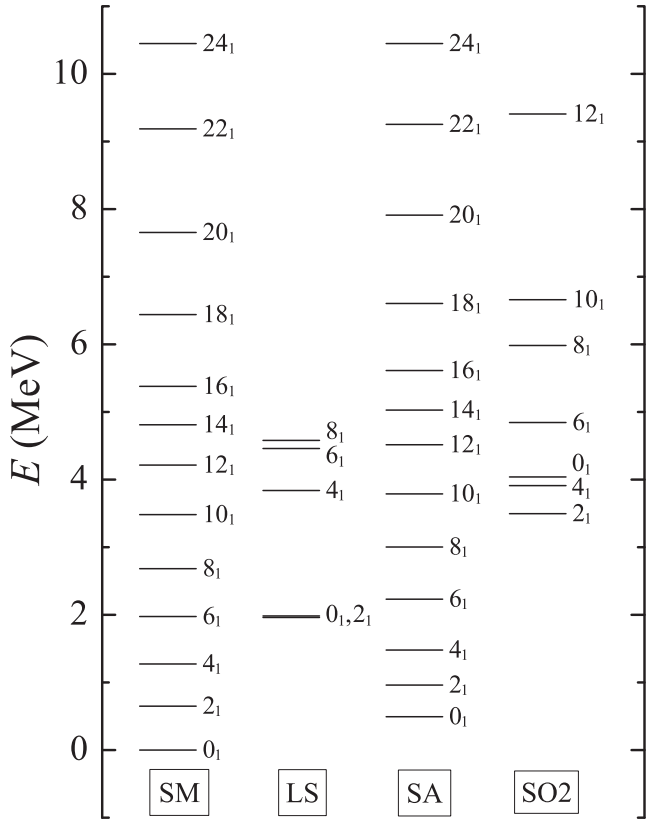

FIG. 4. The yrast states of $T = 0$ for eight nucleons in the $j = 9/2$ shell by using effective interaction (a). "SM" represents the shell model, and the abbreviations "LS", "SA", and "SO2" are the same as in Fig. 1. All the level energies are plotted as relative energies with respect to the 0_1^+ state energy obtained by the SM.

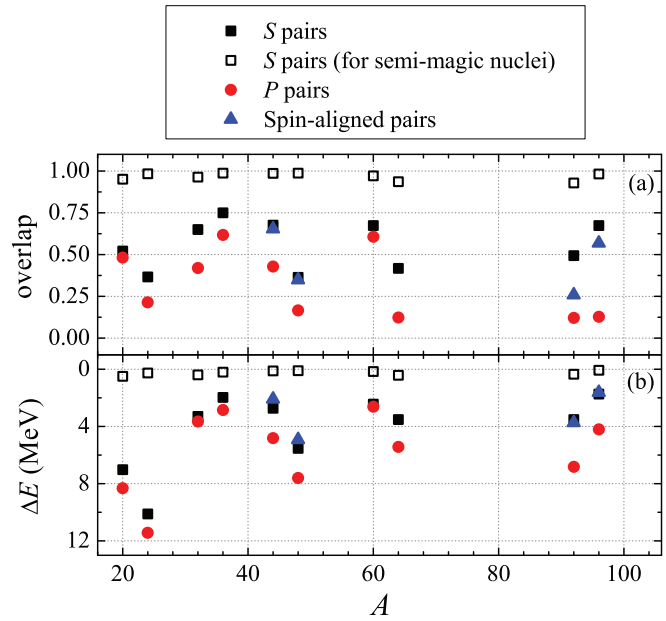

FIG. 5. (Color online) Overlaps between the pair-condensation wave function and the shell-model wave function, and differences between the ground state energy obtained by the pair condensation and that obtained by the shell model, for the ground state of $N = Z$ even-even nuclei by using effective interactions. Solid squares in black represent S pair condensation; solid circles in red represent P pair condensation; solid triangles in blue represent spin-aligned pair condensation. Hallow squares in black represent S pair condensation in semimagic even-even nuclei.

In this section we focus on ground states of ten $N = Z$ even-even nuclei, including four nuclei in the sd shell, ^{20}Ne, ^{24}Mg, ^{32}S, and ^{36}Ar, for which we take the USDB interaction [39], two nuclei in the pf shell, ^{44}Ti and ^{48}Cr, for which we take the GXPF1 interaction [40], and four nuclei in the $p_{1/2}p_{3/2}f_{5/2}g_{9/2}$ shell, ^{60}Zn, ^{64}Ge, ^{92}Pd, and ^{96}Cd, for which we take the JUN45 [41] interaction.

In our previous paper [27] we calculated low-lying states of ^{20}Ne and ^{24}Mg by using various isovector and isoscalar pair approximations. In this paper we study S-pair and P-pair condensations for the ground states. The S-pair condensation wave function is defined in Eq. (3), and the P-pair condensation wave function is defined in Eq. (5). Because the state with $I = 0$ is unique for the P-pair condensation, the calculated result is independent of different choices of intermediate spins in Eq. (5) (the intermediate spin J_2 is equal to either 0 or 2, and J_3 is equal to 1). The nucleon-pair creation operator with spin J_{r_i} and isospin $\mathbb{T}_{r_i}$ for many-j shells is defined by $A^{(r_i)\dagger} = \sum_{j_1 j_2} y(j_1 j_2 r_i)(a_{j_1}{}^{\dagger} \times a_{j_2}{}^{\dagger})^{(r_i)}$, where $y(j_1 j_2 r_i)$ is called pair structure coefficient determined by minimizing the expectation value of Hamiltonian.

We calculate the overlap between the pair-condensation wave function and the SM wave function, for ground states of these $N = Z$ even-even nuclei. We also calculate the energy difference between the binding energy obtained by the pair condensation and that obtained by the shell model (denoted by ΔE). The calculation results are presented in Fig. 5.

It is useful to recall how good S-pair condensation is for ground states of nuclei with same mass numbers but semimagic, ^{20}O, ^{24}O, ^{32}Mg, ^{36}S, ^{44}Ca, ^{48}Ca, ^{60}Ni, ^{64}Ni, ^{92}Mo, and ^{96}Pd. The overlaps between the S-pair condensation wave function and the shell model wave function for these nuclei are plotted in Fig. 5, where one sees that S-pair condensation presents us with a remarkably good truncation scheme. The overlap between the S-pair-condensation wave function and the SM wave function is larger than 0.92, in accordance with the conclusion of the generalized seniority scheme [1]. Interestingly, S-pair condensation is essential in ground states of ^{20}O, ^{36}Ar, ^{44}Ti, ^{60}Zn, and ^{96}Cd, $N = Z$ nuclei with four valence particles (holes). The overlaps are typically $0.52 \sim 0.75$. For the case with eight valence particles (holes), namely here ^{24}Mg, ^{32}S, ^{48}Cr, ^{64}Ge, and ^{92}Pd, the overlap between the S-pair-condensation wave function and the SM wave function decreases by about 0.10, typical overlaps are between 0.36 and 0.65, see solid squares in Fig. 5.

The P-pair condensation is comparably good as the S-pair condensation for ^{20}Ne and ^{60}Zn. For other $N = Z$ nuclei, P-pair condensation presents smaller overlaps with the shell model results, and for ^{24}Mg, ^{48}Cr, ^{64}Ge, ^{92}Pd, and ^{96}Cd, the overlap is below 0.22.

In Ref. [21], low-lying states of ^{92}Pd were calculated in the $p_{1/2}p_{3/2}f_{5/2}g_{9/2}$ shell by using the shell model, and the importance of the spin-aligned pairs was stressed. In the Supplementary Information of Ref. [21], it was reported that the ground state is composed of 95% of the spin-aligned pair truncated wave function. In Refs. [14–20,24–27], low-lying states of ^{92}Pd and ^{96}Cd were studied in the single $g_{9/2}$ shell, and the spin-aligned isoscalar pairs with $J = 9$ was noted to be a key configuration. Similarly, ^{44}Ti and ^{48}Cr were calculated in the single $f_{7/2}$ shell, and the spin-aligned isoscalar pairs with $J = 7$ might present the key configurations [14,25,26]. For these four nuclei, we calculate the ground states in the spin-aligned pair approximation [defined in Eq. (4)], and find that the spin-aligned pair approximation is reasonably good for ^{96}Cd and ^{44}Ti (with four nucleons, see solid triangles in blue in Fig. 5). On the other hand, for nuclei with eight valence particles (holes), ^{92}Pd and ^{48}Cr, the spin-aligned pair approximation is not proper (the overlaps are 0.26 and 0.35, respectively). This is easy to understand, as there is a large probability for valence nucleons (holes) to occupy on orbits other than the $f_{7/2}$ ($g_{9/2}$) orbit for ^{48}Cr (^{92}Pd). Robinson *et al*. calculated low-lying states of ^{44}Ti, ^{48}Cr, ^{88}Ru, ^{92}Pd, and ^{96}Cd in many-j shells by using the shell model, and found the component of the pure $g_{9/2}$-hole configuration in the 0_1^+ and 2_1^+ state wave function of ^{92}Pd is lower than 33% [42]. Neither the result in Ref. [42] nor our result agrees with the Supplementary Information of Ref. [21].

Now we come to the effect of the two-body interactions (with given isospin) on the validity of nucleon-pair approximation. We exemplify this investigation by ground states of ^{24}Mg, ^{48}Cr, and ^{64}Ge, with modified shell model Hamiltonian. We assume two artificial interactions, $H = H_0 + V_{\mathbb{T}=1}$ and $H = H_0 + V_{\mathbb{T}=0}$, i.e., we switch off either the isoscalar or the isovector interactions among the effective interaction parameters. In Fig. 6 one sees that the S-pair condensation for $H = H_0 + V_{\mathbb{T}=1}$ is a much better approximation than for the effective interaction $H_{\rm eff}$, as expected. For $H = H_0 + V_{\mathbb{T}=1}$, the overlaps between the S-pair-condensation wave function and the SM wave function are 0.72, 0.87, and 0.86 for ground states of ^{24}Mg, ^{48}Cr, and ^{64}Ge, respectively. This seems to suggest that the S-pair condensation is not favored for isoscalar interactions. From calculated results shown in Fig. 6, one also sees that the isoscalar P-pair and the isoscalar spin-aligned pair approximation for $H = H_0 + V_{\mathbb{T}=0}$ works better than those for $H_{\rm eff}$, and this suggests that the isoscalar-pair approximations are not favored for isovector interactions. However, there are exceptions to the above naive conjectures; for examples, the S-pair condensation for $H = H_0 + V_{\mathbb{T}=0}$ works better than that for $H_{\rm eff}$ in the ground state of ^{64}Ge; the isoscalar spin-aligned pair approximation for $H = H_0 + V_{\mathbb{T}=1}$ works better than that for $H_{\rm eff}$ in the ground state of ^{48}Cr; the isoscalar P-pair condensation for $H = H_0 + V_{\mathbb{T}=1}$ is superior to that for $H_{\rm eff}$ in the ground state of ^{24}Mg and ^{48}Cr.

References [43–46] suggested that both the isovector and isoscalar pair correlations are suppressed by the spin-orbit coupling potential in medium and heavy nuclei. The isovector pair was defined as a spin-singlet pair with $J = 0$ (total orbital angular momentum $\mathbb{L} = 0$ and total spin $\mathbb{S} = 0$) and $T = 1$,

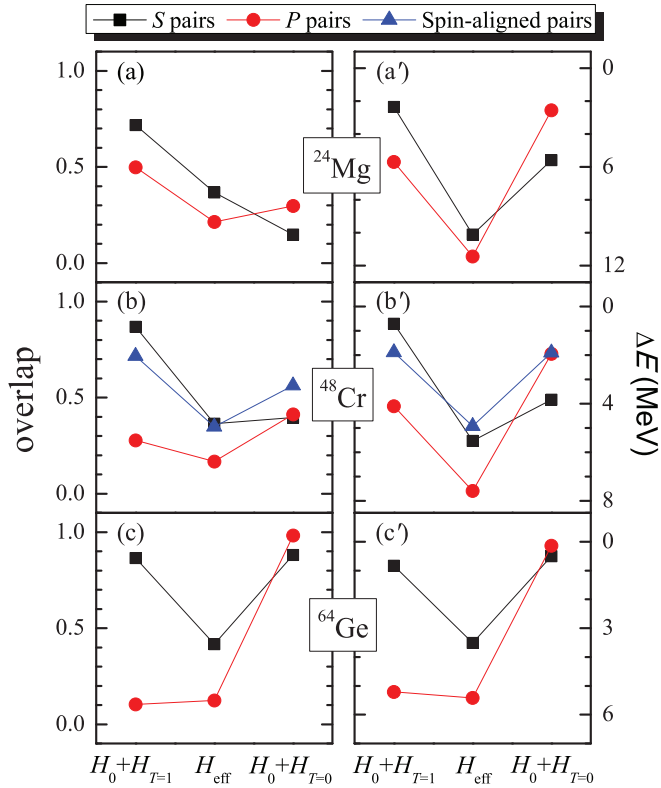

FIG. 6. (Color online) Same as Fig. 5 but for three Hamiltonians, the original effective interaction $H_{\rm eff}$ [Eq. (7)], and two artificial Hamiltonians, one of which switches off the $T = 0$ matrix elements and the other of which switches off the $T = 1$ two-body matrix elements, i.e., $H = H_0 + V_{\mathbb{T}=1}$ and $H_0 + V_{\mathbb{T}=0}$.

and the isoscalar pair was defined as a spin-triplet pair with $J = 1$ ($\mathbb{L} = 0$ and $\mathbb{S} = 1$) and $T = 0$. In this paper we study the effect of the spin-orbit coupling potential on the S-pair and P-pair condensations. The S and P pairs in this paper are slightly different from the isovector and isoscalar pairs in Refs. [43–46] as $\mathbb{L}$ and $\mathbb{S}$ are not good quantum numbers here; the former generalize the latter. We assume a Hamiltonian with parametrized spin-orbit coupling strength,

$$H' = H'_0 + V_{\mathbb{T}=1} + V_{\mathbb{T}=0}, \tag{9}$$

where H'_0 is the modified single-particle energy term in Eq. (8),

$$H'_0 = \sum_j \epsilon'_{nlj} \sum_{m\tau} a_{jm\tau}{}^\dagger a_{jm\tau},$$

and

$$\epsilon'_{nlj} = \epsilon_{nl} - x_{\rm SO} V_{\rm SO} \frac{j(j+1) - l(l+1) - 3/4}{2},$$

$$\epsilon_{nl} = 2\frac{\epsilon_{nl<} - \epsilon_{nl>}}{2l+1},$$

$$V_{\rm SO} = \frac{l\epsilon_{nl<} + (l+1)\epsilon_{nl>}}{2l+1}.$$

Here $\epsilon_{nl<}$ and $\epsilon_{nl>}$ are defined by $\epsilon_{nl<} \equiv \epsilon_{nl(l-\frac{1}{2})}$ and $\epsilon_{nl>} \equiv \epsilon_{nl(l+\frac{1}{2})}$, respectively. $V_{\rm SO}$ is the original spin-orbit coupling potential obtained in the shell model effective Hamiltonian,

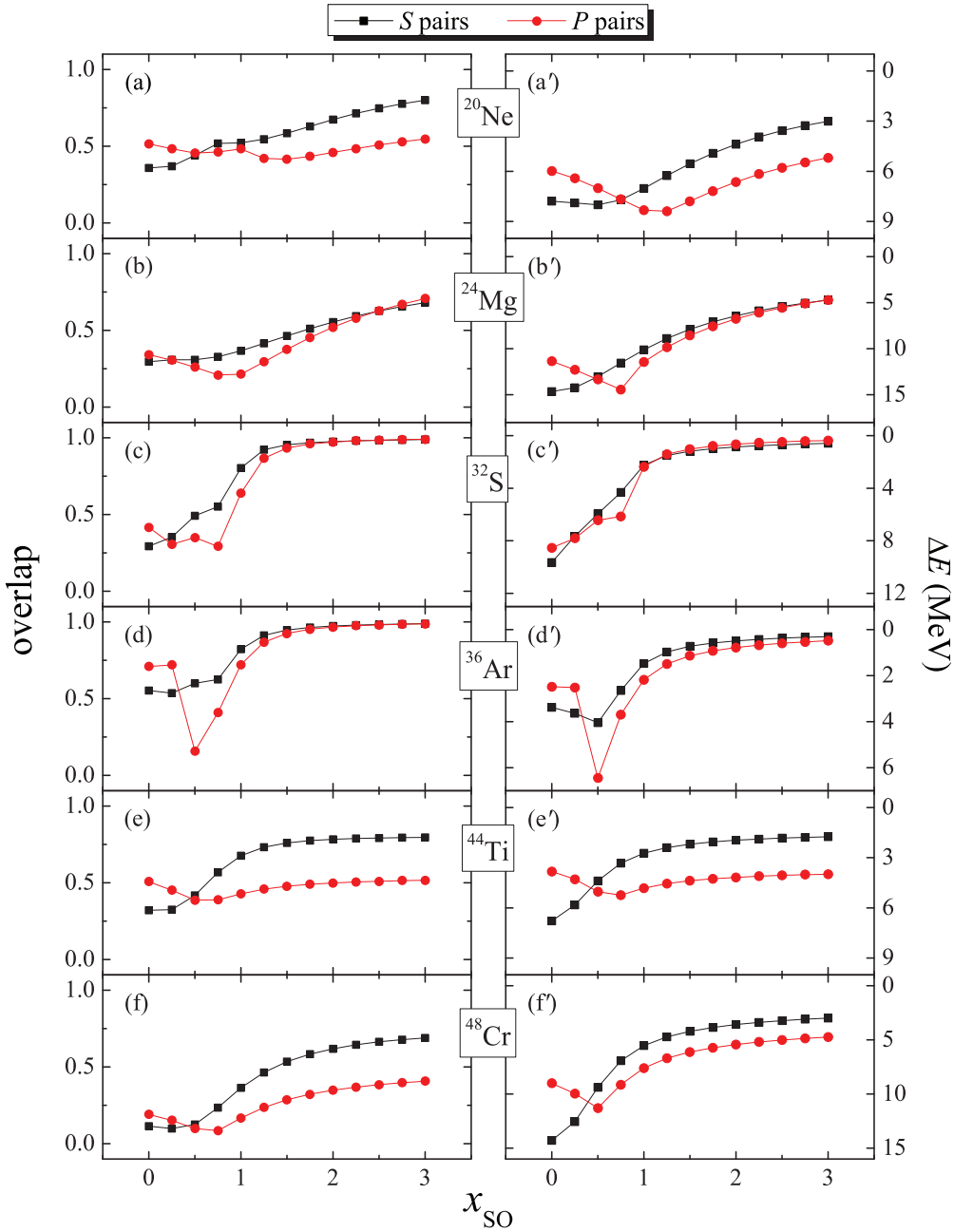

FIG. 7. (Color online) Same as Fig. 5 except that the single-particle energies are reparametrized by x_{SO}, a scale of spin-orbit coupling strength parameter.

and x_{SO} is a parameter we define for the spin-orbit coupling strength ranging between 0 and 3. When $x_{SO} = 1$, H_0' and ϵ_{nlj}' are reduced to H_0 and ϵ_{nlj} in Eq. (8), respectively. Similarly, $x_{SO} = 0$ means no spin-orbit coupling potential; $x_{SO} > 1$ means a stronger spin-orbit coupling potential in H_0' than in H_0; if x_{SO} is large (e.g., $x_{SO} \geqslant 3$), the single-particle energy difference in H_0' is large, and multi-j shells can be approximately represented by a single-j shell.

We study the the ground states of ^{20}Ne, ^{24}Mg, ^{32}S, ^{36}Ar, ^{44}Ti, and ^{48}Cr with the modified effective Hamiltonian H'. We calculate the overlap between the pair-condensation wave functions and the SM wave function, and the difference between the binding energy obtained by the pair condensations and that obtained by the SM, and plot the calculated results in Fig. 7. In general, the overlaps evolve rapidly for $x_{SO} = 0.5$-1, and smoothly for $x_{SO} > 1$. The overlap between the S-pair-condensation wave function and the SM wave function is small at $x_{SO} = 0$, and gradually increases as x_{SO} increases. This behavior of S-pair condensation is consistent with the result in Ref. [47] where S-pair condensation is found to be favored by larger single-particle splittings for semimagic nuclei, ^{22}O and ^{46}Ti, with random interactions. The P-pair condensation is suppressed by the spin-orbit potential in the region with $x_{SO} < 1$. However, it becomes more relevant for $x_{SO} > 1$. The

behavior of the P-pair condensation, as well as the S-pair condensation, is different from Refs. [43–46], in which both the isovector pair correlation and the isoscalar pair correlation are noted to be suppressed by the spin-orbit potential.

Finally, it is worth pointing out that the P-pair condensation works better than S-pair condensation for $x_{\rm SO} \approx 0$. As $x_{\rm SO}$ becomes larger than 0.5, the S-pair condensation is more relevant than P-pair condensation for the ground states of these nuclei.

IV. SUMMARY

In this paper we study isovector and isoscalar pair approximations for low-lying $T = 0$ states of a eight-nucleon system in a single $j = 9/2$ shell and for ground states of $N = Z$ even-even nuclei, ^{20}Ne, ^{24}Mg, ^{32}S, ^{36}Ar, ^{44}Ti, ^{48}Cr, ^{60}Zn, ^{64}Ge, ^{92}Pd, and ^{96}Cd. We present overlaps between wave functions obtained in our various pair-truncated spaces and those obtained in the shell model space.

For eight nucleons in a single $j = 9/2$ shell, the lowest $T = 0$ states with $I = 0,2,\ldots, 8$ are well described by the wave functions with the lowest seniority quantum number with strong $J = 0$ pairing interaction, and are well described by four spin-aligned pairs with strong $J = 2j = 9$ pairing interaction. On the other hand, the low-lying states are not well represented by four P pairs for strong $J = 1$ pairing interaction. The overlap between the wave function with the lowest seniority quantum number and that with spin-aligned pair approximation is $\sim$0.5 for $I = 0$ and 2, and is $\sim$0 for $I = 4,6,8$. The overlap between the P-pair wave function and the lowest-seniority wave function (or the spin-aligned pair wave function) is small. For the yrast $T = 0$ states of eight nucleons in the $g_{9/2}$ shell by using realistic interactions, the spin-aligned pair approximation is very good. If the S pairs and P pairs are further taken into account, the nucleon-pair truncated subspace presents better descriptions.

For the yrast $T = 0$ states of eight nucleons in a single $j = 9/2$ shell, we find that for strong $J = 0$ interaction (the seniority scheme is very good), the $E2$ transition rates of $4^+ \to 2^+$, $6^+ \to 4^+$, and $8^+ \to 6^+$ are close to 0, and the electric-quadrupole moments of the 2^+, 4^+, 6^+, and 8^+ states are very small. When the $J = 2j$ pairing interaction is very strong (the isoscalar spin-aligned pair approximation is very good), the relative $E2$ transition rates of $4^+ \to 2^+$, $6^+ \to 4^+$, and $8^+ \to 6^+$ with respect to $2^+ \to 0^+$ are all approximately equal to 1.5, and the electric-quadrupole moments are all positive (negative) and large for the eight-nucleon (-hole) nucleus. If the $J = 1$ pairing interaction is very strong (the isoscalar P pair approximation is very good), the relative $E2$ transition rates of $4^+ \to 2^+$ and $8^+ \to 6^+$ with respect to $2^+ \to 0^+$ are approximately equal to 2.6 and 3.4, respectively, and that of $6^+ \to 4^+$ is close to 0. The electric-quadrupole moments of the 4^+ and 6^+ states are opposite in signs.

We study ground states of ^{20}Ne, ^{24}Mg, ^{32}S, ^{36}Ar, ^{44}Ti, ^{48}Cr, ^{60}Zn, ^{64}Ge, ^{92}Pd, and ^{96}Cd in multi-j shells. As well known, the S-pair condensation works very well in the case of even-even semimagic nuclei. For even-even $N = Z$ nuclei, the calculated overlap between the S-pair-condensation wave function and the shell model wave function is reasonably large for four valence particles (holes), and becomes smaller for eight valence particles (holes). The P-pair condensation is not good here. The isoscalar spin-aligned pair approximation is good in ^{96}Cd and ^{44}Ti, and is not good in ^{92}Pd and ^{48}Cr. This is different from the single-j shell model results [15–20,25,26]. The reason is that valence holes (nucleons) in ^{92}Pd (^{48}Cr) occupy orbits other than the $g_{9/2}$ ($f_{7/2}$) orbit at large probabilities. By using an artificial interaction without the $T = 0$ ($T = 1$) two-body part, the isovector (isoscalar) pair condensation works better than that with the original effective interaction.

We study the effect of the spin-orbit coupling potential on the isovector and isoscalar pair condensations. We find that the isoscalar P-pair condensation is indeed suppressed in the range that the spin-orbit coupling is weaker than that in effective interactions. When the coupling is stronger, however, isoscalar P pairs become more relevant in the ground state. The isovector S-pair condensation is not good when the spin-orbit coupling is weak, and becomes a better description of the ground state when the coupling is strong. This suggests a different scenario of Refs. [43–46] in which both the correlation of the pair with $J = 0$ ($\mathbb{L} = 0, \mathbb{S} = 0$) and $T = 1$ and the correlation of the pair with $J = 1$ ($\mathbb{L} = 0, \mathbb{S} = 1$) and $T = 0$ are suppressed by the spin-orbit potential.

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