Nucleon-pair approximation with particle-hole excitations

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In this paper, the formalism for the nucleon-pair approximation (NPA) with particle-hole excitations is developed. By using this approach, one is able to perform multiple-major-shell calculations. In this formulation, we use a particle-hole mixed representation, i.e., the particle-hole conjugate transformation is used for operators of the lower major shells, while operators of the upper major shells remain unchanged. We consider collective valence-particle pairs in the upper major shells, collective valence-hole pairs in the lower major shells, and collective pairs consisting of one valence particle in the upper shells and one valence hole in the lower shells to construct our model space. Matrix elements for the shell-model Hamiltonian, both for effective interactions and for phenomenological pairing plus multipole-multipole interactions, are derived in the nucleon-pair basis. As a special case, analytical formulas for doubly magic nuclei with excitations up to two-particle–two-hole are presented. To exemplify this approach, we calculate ^{100}Sn considering both proton and neutron up to four-particle–four-hole excitations, where valence particles are in the 50-82 major shell and valence holes in the 28-50 major shell, with the low-momentum nucleon-nucleon interaction derived from the CD-Bonn potential.

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I. INTRODUCTION

The nuclear shell model (SM) [1,2] is the most fundamental and successful framework in nuclear structure theory. Because of the short-range and attractive nature of nuclear force, pair truncation is one of the most important truncation strategies for the SM space. Significant efforts have been devoted to various pair-truncation schemes, since the early introduction of the seniority scheme [3] and its generalization [4,5], the BCS theory [6–9], the quasispin scheme [10–12] and its generalization [13,14], and the Richardson's model [15,16]. Pair truncation provides the fundamental idea of the successful interacting boson model (IBM) [17], where spin-0 S pairs and spin-2 D pairs are replaced by sd bosons. It has also been applied in a few theoretical models where building blocks are nucleon pairs, such as the broken-pair approximation (BPA) [18,19], the favored-pair model (FPM) [20–22], the weak coupling model of nucleon pairs [23], the multistep shell model [24,25], and two symmetry-dictated models, i.e., the Ginocchio's model [26] and the fermion dynamical symmetry model (FDSM) [27–30]. In the past decade, the (generalized) seniority scheme has been intensively studied; see, e.g., Refs. [31–42].

The nucleon-pair approximation (NPA) is one of the pair-truncation schemes. Chen *et al.* developed a technique to calculate the commutators between coupled operators and between coupled fermion clusters [43,44]. Based on this technique, the formalism of the NPA was suggested and improved in Refs. [45,46]. The building blocks of the NPA are collective nucleon pairs with various spins. If all possible pairs are considered, the NPA goes to the SM; if a very few selected pairs are considered, the SM space is efficiently truncated. The validity of such pair-truncated spaces are studied in different mass regions [47,48]. The model space of the NPA is flexible enough to include the (generalized) seniority scheme, the BPA, the FPM, and the FDSM as special cases. The version of the NPA with isospin symmetry was presented in Ref. [49], where the building blocks are collective pairs with both good spin and good isospin. Numerical studies within the NPA have been performed extensively in the $A = 80$, 100, 130, and 210 regions; see, e.g., Refs. [50–55]. A comprehensive review for the formalism and applications of the NPA can be found in Ref. [56].

Shell-model calculations in multiple major shells have become one of the central themes in nuclear structure theory. Such calculations provide more reliable descriptions for exotic nuclei toward the drip lines, in which the underlying shell structures may evolve substantially with respect to those in stable nuclei [57]. It also plays a key role in the microscopic study of shape coexistence in atomic nuclei [58,59], which may arise from the strong interplay between the low-lying deformed configurations of multiple major shells and spherical configurations of one major shell. Intensive studies for exotic nuclei and nuclear shape coexistence have been performed based on large-scale shell-model (LSSM) calculations and Monte Carlo shell-model (MCSM) calculations; see, e.g., Refs. [60–76]. However, the dramatic increase of the shell-model dimension with the number of active single-j orbits

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prevents the applications of the shell model in the middle-heavy and heavy mass regions. As pointed out in Ref. [59], one has to restrict the model spaces, and a crucial step is to truncate the shell-model basis into a subspace that allows one to treat both low-lying quadrupole excitations and intruder excitations across closed shells; one is able to concentrate on low-lying quadrupole excitations in the NPA, where the general approach to introduce nucleon-pair excitations across closed shells, however, remains to be developed.

In this paper, we propose a formulation to treat particles and holes simultaneously in the NPA, based on which practical multiple-major-shell calculations can be realized. We consider valence particles for the upper major shells and valence holes for the lower ones; thus there are three types of nucleon pairs, i.e., valence-particle pairs in the upper major shells, valence-hole pairs in the lower major shells, and pairs consisting of one valence particle in the upper shells and one valence hole in the lower ones. By considering all three types of pairs, one is able to study not only the role played by nucleon-pair excitations across closed shells, but also the role played by phonons. Technically, the particle-hole conjugate transformation is applied to operators of the lower major shells, while operators of the upper major shells remain unchanged; in other words, we use a "mixed" representation, where the above three types of pairs are allowed to be treated on the same footing.

The paper is organized as follows. In Sec. II, we briefly introduce fundamental operators and coupled commutators, recall particle-hole conjugate transformation, and discuss operators and commutators in the particle-hole mixed representation. In Sec. III, we construct the nucleon-pair configuration space with particle-hole excitations. In Sec. IV, we present formulas for matrix elements of the SM Hamiltonian in the mixed representation. We also derive analytic formulas for doubly magic nuclei with particle-hole excitations up to 2p2h. In Sec. V, we present a numerical study of ^{100}Sn to exemplify the approach proposed in this paper. In Sec. VI, we summarize this paper.

II. FUNDAMENTAL OPERATORS AND COUPLED COMMUTATORS

A. Fundamental operators

In literature, the operator that creates a nucleon in an orbit with quantum numbers n,l,j,m is usually denoted by using $a^{\dagger}_{jm}$. In this paper, for brevity we denote the operator that creates a nucleon with quantum numbers n_a,l_a,j_a,m_a (the a orbit) by using $a^{\dagger} \equiv a^{\dagger}_{j_a m_a}$, and that creates a nucleon in the b orbit by using $b^{\dagger} \equiv a^{\dagger}_{j_b m_b}$. The operator that creates a coupled pair of spin J_e is defined by

$$\begin{aligned} A^{e\dagger} &\equiv A^{J_e\dagger}_{m_e} = \sum_{ab} y(abe) A^{e\dagger}(ab), \\ A^{e\dagger}(ab) &\equiv A^{J_e\dagger}_{m_e}(ab) = (a^{\dagger} \times b^{\dagger})^{J_e}_{m_e}. \end{aligned} \tag{1}$$

Here $(a^{\dagger} \times b^{\dagger})^{J_e}_{m_e} = \sum_{m_a m_b} C^{J_e m_e}_{j_a m_a j_b m_b} a^{\dagger} b^{\dagger}$, and $C^{J_e m_e}_{j_a m_a j_b m_b}$ is a Clebsch-Gordan coefficient. $A^{e\dagger}(ab)$ is called noncollective pair creation operator, and $A^{e\dagger}$ is a collective pair creation operator representing a linear combination of the noncollective pair creation operators with spin J_e. $y(abr)$ is the so-called structure coefficient. From the equation

$$\begin{aligned} A^{e\dagger}(ab) &= -\theta(abe) \times A^{e\dagger}(ba), \\ \theta(abe) &= (-)^{J_e + j_a + j_b}, \end{aligned} \tag{2}$$

one easily obtains a collective pair with structure coefficients satisfying the antisymmetric relation as below:

$$y(abe) = -\theta(abe) y(bae). \tag{3}$$

This antisymmetric relation is used throughout the framework of the NPA.

In literature, the operator that annihilates a nucleon in the orbit with quantum numbers n,l,j,m is defined as $a_{jm} = (a^{\dagger}_{jm})^{\dagger}$. In the NPA, we use the time-reversed form $\tilde{a}_{jm} = (-)^{j-m} a_{j,-m}$, which is a spherical tensor operator of rank j. Again for brevity, we use $\tilde{a}$ and $\tilde{b}$ to denote $\tilde{a}_{j_a m_a}$ and $\tilde{a}_{j_b m_b}$, respectively. The time-reversed form of the operator that annihilates a coupled pair of spin J_e is given by

$$\begin{aligned} \tilde{A}^{e} &\equiv \tilde{A}^{J_e}_{m_e} = \sum_{ab} y(abe) \tilde{A}^{e}(ab), \\ \tilde{A}^{e}(ab) &\equiv \tilde{A}^{J_e}_{m_e}(ab) = -(\tilde{a} \times \tilde{b})^{J_e}_{m_e}. \end{aligned} \tag{4}$$

The collective multipole (particle-hole) operator Q^e represents a linear combination of the noncollective multipole operators with spin J_e, i.e.,

$$\begin{aligned} Q^{e} &\equiv Q^{J_e}_{m_e} = \sum_{ab} q(abe) Q^{e}(ab), \\ Q^{e}(ab) &\equiv Q^{J_e}_{m_e}(ab) = (a^{\dagger} \times \tilde{b})^{J_e}_{m_e}. \end{aligned} \tag{5}$$

Similar to the multipole (particle-hole) operator, in this paper we shall also use collective hole-particle operator O^e and noncollective hole-particle operator $O^e(ab)$, namely,

$$\begin{aligned} O^{e} &\equiv O^{J_e}_{m_e} = \sum_{ab} o(abe) O^{e}(ab), \\ O^{e}(ab) &\equiv O^{J_e}_{m_e}(ab) = (\tilde{a} \times b^{\dagger})^{J_e}_{m_e}. \end{aligned} \tag{6}$$

We can rewrite $O^e(ab)$ and O^e in terms of $Q^e(ba)$,

$$\begin{aligned} O^{e}(ab) &= \delta_{ab}\delta_{e0}\hat{j}_a + (-)^{e-j_a-j_b+1} Q^{e}(ba), \\ O^{e} &= \delta_{e0} \sum_{a} o(aa0)\hat{j}_a + \sum_{ab} (-)^{e-j_a-j_b+1} o(abe) Q^{e}(ba). \end{aligned} \tag{7}$$

Here $\hat{j}_a = \sqrt{2j_a + 1}$.

B. Coupled commutators

Three fundamental commutators in the NPA were given in Ref. [44]. According to Eqs. (3.10a)–(3.10c) and

Eqs. (3.11a)–(3.11c) of Ref. [44],

$$(1)\quad [\tilde{A}^r, A^{s\dagger}]^t = \delta_{rs}\delta_{t0}\left(2\hat{s}\sum_{ab} y(abr)y(abs)\right) - Q^t,$$

$$Q^t = \sum_{da} q(dat)(d^\dagger \times \tilde{a})^t, \quad q(dat) = 4\hat{r}\hat{s}\sum_b y(abr)y(bds)\begin{Bmatrix} j_a & j_b & r \\ s & t & j_d \end{Bmatrix}. \tag{8}$$

$$(2)\quad [\tilde{A}^r, Q^t]^{r'} = \tilde{\mathcal{B}}^{r'} = \sum_{da} y'(dar')\tilde{A}^{r'}(da),$$

$$y'(dar') = z'(dar') - \theta(dar')z'(adr'), \quad z'(dar') = \hat{r}\hat{t}\sum_b y(abr)q(bdt)\begin{Bmatrix} j_a & j_b & r \\ t & r' & j_d \end{Bmatrix}. \tag{9}$$

$$(3)\quad [\tilde{A}^{r_i}, [\tilde{A}^{r_k}, A^{s\dagger}]^t]^{r_i'} = \tilde{\mathcal{B}}^{r_i'} = \sum_{a_1a_2} y'(a_1a_2r_i')\tilde{A}^{r_i'}(a_1a_2), \quad y'(a_1a_2r_i') = z'(a_1a_2r_i') - \theta(a_1a_2r_i')z'(a_2a_1r_i'),$$

$$z'(a_1a_2r_i') = -4\hat{r}_i\hat{r}_k\hat{s}\hat{t}\sum_{b_2b_1} y(a_2b_2r_i)y(a_1b_1r_k)y(b_1b_2s)\begin{Bmatrix} j_{a_2} & j_{b_2} & r_i \\ t & r_i' & j_{a_1} \end{Bmatrix}\begin{Bmatrix} j_{a_1} & j_{b_1} & r_k \\ s & t & j_{b_2} \end{Bmatrix}. \tag{10}$$

Here $\{\begin{smallmatrix} j_a & j_b & r \\ s & t & j_d \end{smallmatrix}\}$ is a 6-j symbol.

In this paper, we shall also need the commutator between the collective pair operator and the collective hole-particle operator defined in Eq. (6). For this commutator, we have

$$[\tilde{A}^r, O^t]^{r'} = \tilde{\mathcal{C}}^{r'} = \sum_{ca} y'(car')\tilde{A}^{r'}(ca),$$
$$y'(car') = z'(car') - \theta(car')z'(acr'), \tag{11}$$
$$z'(car') = \hat{r}\hat{t}\sum_b (-)^{t-j_b-j_c+1} y(abr)o(cbt)\begin{Bmatrix} j_a & j_b & r \\ t & r' & j_c \end{Bmatrix}.$$

C. Particle-hole conjugate transformation

In this subsection, we recall the fundamental particle-hole conjugate transformation (see, e.g., Ref. [77]). We denote the particle-hole conjugation operator as Γ,

$$\Gamma|\text{full}\rangle = |0\rangle, \tag{12}$$

namely, a state of given fully filled shell in the particle representation (denoted as $|\text{full}\rangle$) becomes the vacuum state in the hole representation (denoted as $|0\rangle$) after the operation of Γ; and

$$\Gamma\tilde{a}_{jm}\Gamma^\dagger = a^\dagger_{jm}, \quad \Gamma a^\dagger_{jm}\Gamma^\dagger = -\tilde{a}_{jm}. \tag{13}$$

Equation (13) will be different by a minus sign if one uses the convention of $\tilde{a}_{jm} = (-)^{j+m}a_{j,-m}$ as in Ref. [77].

By using Eq. (13), one obtains the particle-hole conjugate transformation for the coupled commutators of single-particle operators. As shown below, commutators in the hole representation are the same as those in the particle representation:

$$\begin{array}{rcl} \text{particle representation} & & \text{hole representation} \\ (\tilde{a},\tilde{b})^e = 0 & \leftrightarrow & (a^\dagger,b^\dagger)^e = 0, \\ (a^\dagger,b^\dagger)^e = 0 & \leftrightarrow & (\tilde{a},\tilde{b})^e = 0, \\ (\tilde{a},b^\dagger)^e = \ \delta_{e0}\delta_{ab}\hat{j}_a & \leftrightarrow & (a^\dagger,\tilde{b})^e = -\delta_{e0}\delta_{ab}\hat{j}_a, \\ (a^\dagger,\tilde{b})^e = -\delta_{e0}\delta_{ab}\hat{j}_a & \leftrightarrow & (\tilde{a},b^\dagger)^e = \ \delta_{e0}\delta_{ab}\hat{j}_a. \end{array} \tag{14}$$

D. Operators and commutators in the particle-hole mixed representation

Now we apply the particle-hole conjugate transformation to operators of the lower major shells, with operators of the upper major shells unchanged. There are in total four cases for combinations of two orbits a and b:

(1) a,b are both orbits in the upper shells,
(2) a,b are both orbits in the lower shells,
(3) a is an orbit in the upper shells and b is an orbit in the lower shells,
(4) a is an orbit in the lower shells and b is an orbit in the upper shells.

For these four cases, a noncollective pair creation operator and a noncollective pair time-reversal operator, as well as a noncollective multipole operator, in the particle representation are transformed as below:

$$A^{J_e\dagger}_{m_e}(ab) \to A^{J_e\dagger}_{m_e}(ab), \quad -\tilde{A}^{J_e}_{m_e}(ab), \quad -Q^{J_e}_{m_e}(ab), \quad (-)^{J_e-j_a-j_b}Q^{J_e}_{m_e}(ba); \tag{15}$$

$$\tilde{A}^{J_e}_{m_e}(ab) \to \tilde{A}^{J_e}_{m_e}(ab), \quad -A^{J_e\dagger}_{m_e}(ab), \quad (-)^{J_e-j_a-j_b}Q^{J_e}_{m_e}(ba), \quad -Q^{J_e}_{m_e}(ab); \tag{16}$$

$$Q^{J_e}_{m_e}(ab) \to Q^{J_e}_{m_e}(ab), \quad -O^{J_e}_{m_e}(ab), \quad A^{J_e\dagger}_{m_e}(ab), \quad \tilde{A}^{J_e}_{m_e}(ab). \tag{17}$$

If we use i,j to label orbits in the upper shells and μ,ν to label orbits in the lower shells, respectively, a collective pair creation operator and a collective pair time-reversal operator, as well as a collective multipole operator, in the particle representation are transformed as below,

$$A^{J_e\dagger}_{m_e} \to \sum_{ij} y(ije)A^{J_e\dagger}_{m_e}(ij) - \sum_{\mu\nu} y(\mu\nu e)\tilde{A}^{J_e}_{m_e}(\mu\nu) - \sum_{i\mu}[y(i\mu e) - (-)^{J_e-j_i-j_\mu}y(\mu i e)]Q^{J_e}_{m_e}(i\mu); \tag{18}$$

$$\tilde{A}^{J_e}_{m_e} \rightarrow \sum_{ij} y(ije)\tilde{A}^{J_e}_{m_e}(ij) - \sum_{\mu\nu} y(\mu\nu e)A^{J_e\dagger}_{m_e}(\mu\nu) - \sum_{i\mu}[y(\mu ie) - (-)^{J_e-j_i-j_\mu}y(i\mu e)]Q^{J_e}_{m_e}(\mu i); \quad (19)$$

$$Q^{J_e}_{m_e} \rightarrow \sum_{ij} q(ije)Q^{J_e}_{m_e}(ij) - \sum_{\mu\nu} q(\mu\nu e)O^{J_e}_{m_e}(\mu\nu) + \sum_{i\mu} q(i\mu e)A^{J_e\dagger}_{m_e}(i\mu) + \sum_{\mu i} q(\mu ie)\tilde{A}^{J_e}_{m_e}(\mu i). \quad (20)$$

For basic commutators of single-particle operators, there are three cases in the mixed representation as follows:

(1) Both orbits of two operators are in the upper major shells; in this case the coupled commutators are given by the left column in Eq. (14).
(2) Both orbits of two operators are in the lower major shells; in this case the coupled commutators are described in the right column in Eq. (14).
(3) One orbit is in the upper major shells and the other is in the lower major shells; the commutators are necessarily zero.

Therefore, all commutators in the particle representation presented in Sec. II.B, namely Eqs. (8)–(11), also hold in this particle-hole mixed representation.

III. COLLECTIVE PAIR BASIS IN THE PARTICLE-HOLE MIXED REPRESENTATION

In the mixed representation, there are three types of nucleon pairs: particle-particle (pp) pairs consisting of two valence particles in the upper major shells, hole-hole (hh) pairs consisting of two valence holes in the lower major shells, and particle-hole (ph) pairs consisting of one valence particle in the upper shells and one valence hole in the lower ones. The operators that create collective pp, hh, and ph pairs are given by the first term of Eq. (18), the second term of Eq. (19), and the third term of Eq. (20), respectively. Let us use $j_1, j_2, \ldots, j_n$ to label orbits in the upper major shells and $j_{n+1}, j_{n+2}, \ldots, j_{n+m}$ to label orbits in the lower major shells. The structure coefficients of pp, hh, and ph pair creation operators are then in the form as follows:

$$y_{\rm pp} = \begin{pmatrix} A_{n\times n} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad y_{\rm hh} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_{m\times m} \end{pmatrix}, \quad y_{\rm ph} = \begin{pmatrix} \mathbf{0} & C_{n\times m} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}. \quad (21)$$

Here the subscripts "pp," "hh," and "ph" correspond to pp, hh, and ph pairs, respectively. In the NPA, the above structure coefficients should be modified to satisfy the antisymmetric relation, namely Eq. (3).

According to Eq. (12), the vacuum state $|0\rangle$ in the mixed representation is the state of the fully filled lower major shells. Pair basis states are constructed by collective pair creation operators coupled successively and acting on the vacuum state. The particle number conservation constrains the number of pp pairs and that of hh pairs in a basis state (denoted as $N_{\rm pp}$ and $N_{\rm hh}$, respectively). Let us assume that Ω_0 is the capacity of the lower major shells for like nucleons, i.e., $\Omega_0 = \sum_{i=n+1}^{n+m}(2j_i+1)$. We have

$$N_{\rm pp} - N_{\rm hh} = \begin{cases} N, & \text{for a system with } \Omega_0 + 2N \text{ (or } \Omega_0 + 2N + 1\text{) like nucleons;} \\ -N', & \text{for a system with } \Omega_0 - 2N' \text{ (or } \Omega_0 - 2N' - 1\text{) like nucleons;} \\ 0, & \text{for a system with } \Omega_0 \text{ (or } \Omega_0 \pm 1\text{) like nucleons.} \end{cases} \quad (22)$$

Next, we use two examples with particle-hole excitations up to 2p2h to exemplify our pair configuration space. For a system with even particle number that is larger than Ω_0, e.g., a system of $(\Omega_0 + 2N)$ like nucleons, the configuration space includes four kinds of pair basis states as below:

$$\begin{aligned} &\big[\big(A^{r_1\dagger}_{\rm pp} \times A^{r_2\dagger}_{\rm pp}\big)^{(J_2)} \times \cdots \times A^{r_N\dagger}_{\rm pp}\big]^{(J_N)}|0\rangle, \\ &\big\{\big[\big(A^{r_1\dagger}_{\rm pp} \times A^{r_2\dagger}_{\rm pp}\big)^{(J_2)} \times \cdots \times A^{r_N\dagger}_{\rm pp}\big]^{(J_N)} \times A^{r_{N+1}\dagger}_{\rm ph}\big\}^{(J_{N+1})}|0\rangle, \\ &\big(\big\{\big[\big(A^{r_1\dagger}_{\rm pp} \times A^{r_2\dagger}_{\rm pp}\big)^{(J_2)} \times \cdots \times A^{r_N\dagger}_{\rm pp}\big]^{(J_N)} \times A^{r_{N+1}\dagger}_{\rm ph}\big\}^{(J_{N+1})} \times A^{r_{N+2}\dagger}_{\rm ph}\big)^{(J_{N+2})}|0\rangle, \\ &\big(\big\{\big[\big(A^{r_1\dagger}_{\rm pp} \times A^{r_2\dagger}_{\rm pp}\big)^{(J_2)} \times \cdots \times A^{r_N\dagger}_{\rm pp}\big]^{(J_N)} \times A^{r_{N+1}\dagger}_{\rm pp}\big\}^{(J_{N+1})} \times A^{r_{N+2}\dagger}_{\rm hh}\big)^{(J_{N+2})}|0\rangle. \end{aligned} \quad (23)$$

For a system with odd particle number that is smaller than Ω_0, e.g., a system with $(\Omega_0 - 2N' - 1)$ nucleons, the configuration space includes similarly four kinds of pair basis states:

$$\begin{aligned} &\big\{\big[\big(a^{\dagger}_{j_{\rm h}} \times A^{r_1\dagger}_{\rm hh}\big)^{(J_1)} \times A^{r_2\dagger}_{\rm hh}\big]^{(J_2)} \times \cdots \times A^{r_{N'}\dagger}_{\rm hh}\big\}^{(J_{N'})}|0\rangle, \\ &\big(\big\{\big[\big(a^{\dagger}_{j_{\rm h}} \times A^{r_1\dagger}_{\rm hh}\big)^{(J_1)} \times A^{r_2\dagger}_{\rm hh}\big]^{(J_2)} \times \cdots \times A^{r_{N'}\dagger}_{\rm hh}\big\}^{(J_{N'})} \times A^{r_{N'+1}\dagger}_{\rm ph}\big)^{(J_{N'+1})}|0\rangle, \\ &\big[\big(\big\{\big[\big(a^{\dagger}_{j_{\rm h}} \times A^{r_1\dagger}_{\rm hh}\big)^{(J_1)} \times A^{r_2\dagger}_{\rm hh}\big]^{(J_2)} \times \cdots \times A^{r_{N'}\dagger}_{\rm hh}\big\}^{(J_{N'})} \times A^{r_{N'+1}\dagger}_{\rm ph}\big)^{(J_{N'+1})} \times A^{r_{N'+2}\dagger}_{\rm ph}\big]^{(J_{N'+2})}|0\rangle, \\ &\big[\big(\big\{\big[\big(a^{\dagger}_{j_{\rm h}} \times A^{r_1\dagger}_{\rm hh}\big)^{(J_1)} \times A^{r_2\dagger}_{\rm hh}\big]^{(J_2)} \times \cdots \times A^{r_{N'}\dagger}_{\rm hh}\big\}^{(J_{N'})} \times A^{r_{N'+1}\dagger}_{\rm hh}\big)^{(J_{N'+1})} \times A^{r_{N'+2}\dagger}_{\rm pp}\big]^{(J_{N'+2})}|0\rangle. \end{aligned} \quad (24)$$

Here the subscript $j_{\rm h}$ labels an orbit in the lower shells.

In Eq. (23), the basis states of $N, N+1, N+2$ pairs correspond to 0p0h, 1p1h, and 2p2h excitations, respectively. One easily sees the overlap between one basis state of $N+n$ pairs (corresponding to the npnh excitation) and the other of $N+n'$ pairs (corresponding to the n'pn'h excitation) vanishes unless $n = n'$. If we define

$$\begin{aligned}&\langle r_1 \dots r_N, J_1 \dots J_N M_N| \\ &\quad = \langle 0|(-)^{J_N+M_N}[(\tilde{A}^{r_1} \times \tilde{A}^{r_2})^{(J_2)} \times \cdots \times \tilde{A}^{r_N}]^{(J_N)}_{-M_N}, \\ &|s_1 \dots s_{N'}, J_1' \dots J_{N'}' M_{N'}'\rangle \\ &\quad = [(A'^{s_1\dagger} \times A'^{s_2\dagger})^{(J_2')} \times \cdots \times A'^{s_{N'}\dagger}]^{(J_{N'}')}_{M_{N'}'}|0\rangle,\end{aligned}$$

the overlap between them is given by

$$\begin{aligned}&\langle r_1 \dots r_N, J_1 \dots J_N M_N | s_1 \dots s_{N'}, J_1' \dots J_{N'}' M_{N'}'\rangle \\ &\quad = \delta_{NN'}\langle r_1 \dots r_N, J_1 \dots J_N M_N | s_1 \dots s_N, J_1' \dots J_N' M_N'\rangle.\end{aligned} \tag{25}$$

Similarly, the overlap for an odd-number system vanishes unless $n = n'$. The overlap in the right-hand side of the above equation can be calculated by using recursive formulas in Refs. [45,46].

Clearly, if all possible pp, hh, and ph pairs are considered, our nucleon-pair configuration space up to npnh excitations constructed above is equivalent to the exact SM space of particle-hole excitations up to npnh. If only a very few collective pp, hh, and ph pairs are selected, the SM space is tremendously truncated.

IV. MATRIX ELEMENTS IN THE PARTICLE-HOLE MIXED REPRESENTATION

In this section, we derive matrix elements of the SM Hamiltonian in the nucleon-pair basis constructed in Sec. III. For doubly magic nuclei with particle-hole excitations up to 2p2h, we also give analytical expressions as a special case of the present formulation.

A. Shell-model Hamiltonians

In the SM studies, two forms of the Hamiltonian H, with either effective interactions or phenomenological paring plus multipole-multipole interactions, are usually adopted. H with effective interactions is

$$H = \sum_j \varepsilon_j N_j + \sum_{j_1 \leqslant j_2} \sum_{j_3 \leqslant j_4} \sum_{JM} \sum_{TM_T} \frac{V_{JT}(j_1 j_2 j_3 j_4)}{\sqrt{(1+\delta_{j_1 j_2})(1+\delta_{j_3 j_4})}} A^{JT\dagger}_{MM_T}(j_1 j_2) A^{JT}_{MM_T}(j_3 j_4). \tag{26}$$

Here $N_j = \sum_{m\tau} a^\dagger_{jm\frac{1}{2}\tau} a_{jm\frac{1}{2}\tau}$; the pair creation operator and the pair annihilation operator with both good spin J and good isospin T are given by

$$\begin{aligned}A^{JT\dagger}_{MM_T}(j_1 j_2) &= \sum_{m_1 m_2} \sum_{\tau_1 \tau_2} C^{JM}_{j_1 m_1 j_2 m_2} C^{TM_T}_{\frac{1}{2}\tau_1 \frac{1}{2}\tau_2} a^\dagger_{j_1 m_1 \frac{1}{2}\tau_1} a^\dagger_{j_2 m_2 \frac{1}{2}\tau_2}, \\ A^{JT}_{MM_T}(j_3 j_4) &= -\sum_{m_3 m_4} \sum_{\tau_3 \tau_4} C^{JM}_{j_3 m_3 j_4 m_4} C^{TM_T}_{\frac{1}{2}\tau_3 \frac{1}{2}\tau_4} a_{j_3 m_3 \frac{1}{2}\tau_3} a_{j_4 m_4 \frac{1}{2}\tau_4},\end{aligned}$$

with $C^{JM}_{j_1 m_1 j_2 m_2}$ and $C^{TM_T}_{\frac{1}{2}\tau_1 \frac{1}{2}\tau_2}$ being Clebsch-Gordan coefficients. In the above Hamiltonian, the two-body interactions $V_{JT}(j_1 j_2 j_3 j_4)$ can be either derived microscopically from the realistic nuclear force [78–82] or obtained by fitting to experimental data in a shell region [83–86].

In the NPA, we separate the above Hamiltonian into the proton part, neutron part, and proton-neutron part, namely,

$$\begin{aligned}H &= \sum_{\sigma=\pi,\nu} H_\sigma + H_{\pi\nu}, \\ H_\sigma &= \sum_j \varepsilon_j n_{j\sigma} + \sum_{j_1 \leqslant j_2} \sum_{j_3 \leqslant j_4} \sum_J \frac{V_{JT=1}(j_1 j_2 j_3 j_4)}{\sqrt{(1+\delta_{j_1 j_2})(1+\delta_{j_3 j_4})}} \hat{J}\big[A^{J\dagger}_\sigma(j_1 j_2) \times \tilde{A}^J_\sigma(j_3 j_4)\big]^{(0)}, \\ H_{\pi\nu} &= -\sum_{j_1 j_2} \sum_{j_3 j_4} \sum_J V^{\pi\nu}_J(j_1 j_2 j_3 j_4) \hat{J}\big[\big(a^\dagger_{j_1\pi} \times a^\dagger_{j_2\nu}\big)^J \times \big(\tilde{a}_{j_3\pi} \times \tilde{a}_{j_4\nu}\big)^J\big]^{(0)}, \\ V^{\pi\nu}_J(j_1 j_2 j_3 j_4) &= \frac{1}{2}[V_{JT=1}(j_1 j_2 j_3 j_4) + V_{JT=0}(j_1 j_2 j_3 j_4)]\sqrt{(1+\delta_{j_1 j_2})(1+\delta_{j_3 j_4})}.\end{aligned} \tag{27}$$

Here $n_{j\sigma} = \sum_m (a^\dagger_{jm})_\sigma (a_{jm})_\sigma$. To calculate matrix elements of the above $H_{\pi\nu}$ in the NPA, we further express $H_{\pi\nu}$ in terms of proton-neutron multipole-multipole interactions. Denoting $j_{1\pi} \equiv j_\pi$, $j_{2\nu} \equiv j_\nu$, $j_{3\pi} \equiv j'_\pi$, $j_{4\nu} \equiv j'_\nu$, we have

$$H_{\pi\nu} = \sum_{j_\pi j'_\pi} \sum_{j_\nu j'_\nu} \sum_k \left[\sum_J (-)^{J+j_\nu+j'_\pi}(2J+1)\begin{Bmatrix} j_\pi & j_\nu & J \\ j'_\nu & j'_\pi & k\end{Bmatrix} V^{\pi\nu}_J(j_\pi j_\nu j'_\pi j'_\nu)\right](-)^k \hat{k}[Q^k(j_\pi j'_\pi) \times Q^k(j_\nu j'_\nu)]^{(0)}. \tag{28}$$

The matrix elements of $[Q^k(j_\pi j'_\pi) \times Q^k(j_\nu j'_\nu)]^{(0)}$ are calculated using $\langle \alpha_\pi J_\pi \| Q^k(j_\pi j'_\pi) \| \alpha'_\pi J'_\pi\rangle$ and $\langle \alpha_\nu J_\nu \| Q^k(j_\nu j'_\nu) \| \alpha'_\nu J'_\nu\rangle$.

The Hamiltonian with phenomenological pairing and multipole-multipole interactions is

$$\begin{aligned} H &= \sum_{\sigma=\pi,\nu} H_\sigma + H_{\pi\nu}, \\ H_\sigma &= \sum_j \varepsilon_j n_{j\sigma} + \sum_{s=0,2} G_s \hat{s}\big(A_\sigma^{s\dagger} \times \tilde{A}_\sigma^s\big)^{(0)} + \sum_t \kappa_t \hat{t}\big(Q_\sigma^t \times Q_\sigma^t\big)^{(0)}, \\ H_{\pi\nu} &= \sum_t \kappa_t^{\pi\nu} \hat{t}\big(Q_\pi^t \times Q_\nu^t\big)^{(0)}, \end{aligned} \tag{29}$$

where G_s, κ_t, and $\kappa_t^{\pi\nu}$ are strength parameters adjusted in reasonable ranges to achieve an optimal agreement with experimental energy levels and electromagnetic properties.

B. One-body matrix elements in the mixed representation

In this subsection, we discuss reduced matrix elements of the collective multipole operator Q^t. The operator Q^t in the particle representation is transformed into $Q^t + O^t + A^{t\dagger} + \tilde{A}^t$ in the mixed representation, with the structure coefficients describe in Eq. (20). For brevity, we denote in this paper

$$U_1 = Q^t, \quad U_2 = O^t, \quad U_3 = A^{t\dagger}, \quad U_4 = \tilde{A}^t. \tag{30}$$

The reduced matrix element of $U_1 = Q^t$ is given by

$$U_1 : \langle r_1 \dots r_N, J_1 \dots J_N \| Q^t \| s_1 \dots s_{N'}, J'_1 \dots J'_{N'} \rangle = \delta_{NN'} \langle r_1 \dots r_N, J_1 \dots J_N \| Q^t \| s_1 \dots s_N, J'_1 \dots J'_N \rangle. \tag{31}$$

To calculate the right-hand side of Eq. (31), recursive formulas were given in Refs. [45,46].

Reduced matrix elements for the other three one-body operators, O^t (with the structure coefficients denoted as o), $A^\dagger$, and $\tilde{A}$, are given in terms of overlaps and reduced matrix elements of Q^t as follows:

$$\begin{aligned} &U_2 : \langle r_1 \dots r_N, J_1 \dots J_N \| O^t \| s_1 \dots s_{N'}, J'_1 \dots J'_{N'} \rangle \\ &\quad = \delta_{NN'} \left\{ \delta_{t0} \left(\sum_a o(aa0) \hat{j}_a \right) \langle r_1 \dots r_N, J_1 \dots J_N | s_1 \dots s_{N'}, J'_1 \dots J'_{N'} \rangle + \langle r_1 \dots r_N, J_1 \dots J_N \| Q^t \| s_1 \dots s_{N'}, J'_1 \dots J'_{N'} \rangle \right\}, \\ &Q^t = \sum_{ba} q(bat)(b^\dagger \times \tilde{a})^t, \quad q(bat) = (-)^{t-j_a-j_b+1} o(abt); \end{aligned} \tag{32}$$

$$\begin{aligned} &U_3 : \langle r_1 \dots r_N, J_1 \dots J_N \| A^{t\dagger} \| s_1 \dots s_{N'}, J'_1 \dots J'_{N'} \rangle = \delta_{N(N'+1)} \langle r_1 \dots r_N, J_1 \dots J_N | s_1 \dots s_{N'}(t)_A, J'_1 \dots J'_{N'} J_N \rangle, \\ &|s_1 \dots s_{N'}(t)_A, J'_1 \dots J'_{N'} J_N M_N \rangle = \{[(A'^{s_1\dagger} \times A'^{s_2\dagger})^{(J'_2)} \times \dots \times A'^{s_{N'}\dagger}]^{(J'_{N'})} \times A^{t\dagger}\}^{(J_N)}_{M_N} |0\rangle; \end{aligned} \tag{33}$$

$$\begin{aligned} &U_4 : \langle r_1 \dots r_N, J_1 \dots J_N \| \tilde{A}^t \| s_1 \dots s_{N'}, J'_1 \dots J'_{N'} \rangle = \delta_{(N+1)N'} (-)^{J'_{N'} - J_N - t} \frac{\hat{J'}_{N'}}{\hat{J}_N} \langle r_1 \dots r_N(t)_A, J_1 \dots J_N J'_{N'} | s_1 \dots s_{N'}, J'_1 \dots J'_{N'} \rangle, \\ &\langle r_1 \dots r_N(t)_A, J_1 \dots J_N J'_{N'} M'_{N'} | = \langle 0 | (-)^{J'_{N'} + M'_{N'}} \{[(\tilde{A}^{r_1} \times \tilde{A}^{r_2})^{(J_2)} \times \dots \times \tilde{A}^{r_N}]^{(J_N)} \times \tilde{A}^t\}^{(J'_{N'})}_{-M'_{N'}}. \end{aligned} \tag{34}$$

As shown above, considering bra vectors of npnh excitations and ket vectors of n'pn'h excitations, U_1 and U_2 have nonzero matrix elements when $n = n'$, and U_3 and U_4 have nonzero matrix elements when $n = n' + 1$ and $n' = n + 1$, respectively. We also present the distribution of nonzero matrix elements for U_1,...,U_4 in Fig. 1(a). In this paper, we use the convention of $\langle \alpha J M | Q^t_\tau | \alpha' J' M' \rangle = C^{JM}_{J'M' t\tau} \langle \alpha J \| Q^t \| \alpha' J' \rangle$ for reduced matrix elements.

C. Two-body matrix elements in the mixed representation

For brevity, we denote

$$\begin{aligned} V_1 &= \big(A_1^{t\dagger} \times \tilde{A}_2^t\big)^{(0)}, \quad V_2 = \big(Q_1^t \times Q_2^t\big)^{(0)}, \\ V_3 &= \big(\tilde{A}_1^t \times A_2^{t\dagger}\big)^{(0)}, \quad V_4 = \big(O_1^t \times O_2^t\big)^{(0)}, \\ V_5 &= (Q^t \times O^t)^{(0)}, \quad V_6 = (O^t \times Q^t)^{(0)}, \\ V_7 &= (\tilde{A}^t \times Q^t)^{(0)}, \quad V_8 = (Q^t \times \tilde{A}^t)^{(0)}, \\ V_9 &= (\tilde{A}^t \times O^t)^{(0)}, \quad V_{10} = (O^t \times \tilde{A}^t)^{(0)}, \\ V_{11} &= \big(\tilde{A}_1^t \times \tilde{A}_2^t\big)^{(0)}, \quad V_{12} = \big(A_1^{t\dagger} \times A_2^{t\dagger}\big)^{(0)}, \\ V_{13} &= (A^{t\dagger} \times Q^t)^{(0)}, \quad V_{14} = (Q^t \times A^{t\dagger})^{(0)}, \\ V_{15} &= (A^{t\dagger} \times O^t)^{(0)}, \quad V_{16} = (O^t \times A^{t\dagger})^{(0)}. \end{aligned} \tag{35}$$

A collective pair creation operator $A^{t\dagger}$ (or a collective pair time-reversal operator $\tilde{A}^t$) in the particle representation is transformed into $U_1 + U_3 + U_4$ in the mixed representation, with structure coefficients described in Eq. (18) [or Eq. (19)]. Therefore, $(A_1^{t\dagger} \times \tilde{A}_2^t)^{(0)}$ in the particle representation is transformed into $V_1 + V_2 + V_3 + V_7 + V_8 + V_{11} + V_{12} + V_{13} + V_{14}$. Because a collective multipole operator Q^t

(a)

	0p0h	1p1h	2p2h	3p3h	……
0p0h	1,2	4			
1p1h	3	1,2	4		
2p2h		3	1,2	4	
3p3h			3	1,2	
……					

(b)

	0p0h	1p1h	2p2h	3p3h	……
0p0h	1,...,6	7,...,10	11		
1p1h	13,...,16	1,...,6	7,...,10	11	
2p2h	12	13,...,16	1,...,6	7,...,10	
3p3h		12	13,...,16	1,...,6	
……					

FIG. 1. Distributions of nonzero matrix elements for (a) U_i with $i = 1,2,3,4$ and for (b) V_j with $j = 1,...,16$. The bra vectors of the matrix elements in the first, second, third, fourth, etc. rows correspond to 0p0h, 1p1h, 2p2h, 3p3h, etc. excitations, respectively. The ket vectors of the matrix elements in the first, second, third, fourth, etc. columns correspond to 0p0h, 1p1h, 2p2h, 3p3h, etc. excitations, respectively.

in the particle representation is transformed into $U_1 + U_2 + U_3 + U_4$, with structure coefficients described in Eq. (20), the two-body operator $(Q_1^t \times Q_2^t)^{(0)}$ is transformed into the sum of all sixteen V_i in Eq. (35). In Fig. 1(b), we present the distribution of nonzero matrix elements for $V_1,...,V_{16}$. Considering bra vectors of npnh excitations and ket vectors of $n'pn'$h excitations, $V_1,...,V_6$ have nonzero matrix elements when $n = n'$. $V_7,...,V_{10}$ and $V_{13},...,V_{16}$ have nonzero matrix elements when $n' = n + 1$ and $n = n' + 1$, respectively. V_{11} and V_{12} have nonzero matrix elements when $n' = n + 2$ and $n = n' + 2$, respectively.

Because the Hamiltonian is Hermitian, we need only up-triangle matrix elements in Fig. 1(b), namely, results of $V_1,...,V_{11}$. Among these operators, $V_1 = (A_1^{t\dagger} \times \tilde{A}_2^t)^{(0)}$ and $V_2 = (Q_1^t \times Q_2^t)^{(0)}$ are computed by using recursive formulas of Refs. [45,46]. Below we present formulas for matrix elements of $V_3,...,V_{11}$ in terms of overlaps, the reduced matrix element of Q^t, and the matrix elements of $(A_1^{t\dagger} \times \tilde{A}_2^t)^{(0)}$ and $(Q_1^t \times Q_2^t)^{(0)}$. With the help of Eq. (8), we have the formula for matrix elements of $V_3 = (\tilde{A}_1^t \times A_2^{t\dagger})^{(0)}$ (the structure coefficients of $\tilde{A}_1^t$ and $A_2^{t\dagger}$ are denoted as y_1 and y_2),

$$
\begin{aligned}
V_3 :\ & \langle r_1 \ldots r_N, J_1 \ldots J_N | \big(\tilde{A}_1^t \times A_2^{t\dagger}\big)^{(0)} | s_1 \ldots s_{N'}, J_1' \ldots J_{N'}' \rangle \\
&= \delta_{NN'} \delta_{J_N J_{N'}'} \Bigg\{ \Bigg(2\hat{t} \sum_{ab} y_1(abt) y_2(abt) \Bigg) \langle r_1 \ldots r_N, J_1 \ldots J_N | s_1 \ldots s_{N'}, J_1' \ldots J_{N'}' \rangle \\
&\quad - \langle r_1 \ldots r_N, J_1 \ldots J_N \| Q^{(0)} \| s_1 \ldots s_{N'}, J_1' \ldots J_{N'}' \rangle + \langle r_1 \ldots r_N, J_1 \ldots J_N | \big(A_2^{t\dagger} \times \tilde{A}_1^t\big)^{(0)} | s_1 \ldots s_{N'}, J_1' \ldots J_{N'}' \rangle \Bigg\}, \\
Q^{(0)} &= \sum_{da} q(da0) (d^\dagger \times \tilde{a})^{(0)}, \quad q(da0) = \delta_{j_d j_a} \frac{4\hat{t}}{\hat{j}_a} \sum_b (-)^{j_a + j_b + t} y_1(abt) y_2(bdt).
\end{aligned}
\tag{36}
$$

V_4, V_5, V_6 involve the operator O^t. Based on Eq. (7), we have the formula for matrix elements of $V_4 = (O_1^t \times O_2^t)^{(0)}$ (the structure coefficients of O_1^t and O_2^t are denoted as o_1 and o_2),

$$
\begin{aligned}
V_4 :\ & \langle r_1 \cdots r_N, J_1 \cdots J_N | \big(O_1^t \times O_2^t\big)^{(0)} | s_1 \cdots s_{N'}, J_1' \cdots J_{N'}' \rangle \\
&= \delta_{NN'} \delta_{J_N J_{N'}'} \Bigg\{ \delta_{t0} \Bigg(\sum_a o_1(aa0) \hat{j}_a \Bigg) \Bigg(\sum_c o_2(cc0) \hat{j}_c \Bigg) \langle r_1 \ldots r_N, J_1 \ldots J_N | s_1 \ldots s_{N'}, J_1' \ldots J_{N'}' \rangle \\
&\quad + \delta_{t0} \Bigg(\sum_a o_1(aa0) \hat{j}_a \Bigg) \langle r_1 \ldots r_N, J_1 \ldots J_N \| Q_2^{(0)} \| s_1 \ldots s_{N'}, J_1' \ldots J_{N'}' \rangle \\
&\quad + \delta_{t0} \Bigg(\sum_c o_2(cc0) \hat{j}_c \Bigg) \langle r_1 \ldots r_N, J_1 \ldots J_N \| Q_1^{(0)} \| s_1 \ldots s_{N'}, J_1' \ldots J_{N'}' \rangle
\end{aligned}
$$

$$+\langle r_1\dots r_N,J_1\dots J_N|\big(Q_1^t\times Q_2^t\big)^{(0)}|s_1\dots s_{N'},J_1'\dots J_{N'}'\rangle\Bigg\},$$
$$Q_1^t=\sum_{ba}q_1(bat)(b^\dagger\times\tilde{a})^t,\quad q_1(bat)=(-)^{t-j_a-j_b+1}o_1(abt),$$
$$Q_2^t=\sum_{dc}q_2(dct)(d^\dagger\times\tilde{c})^t,\quad q_2(dct)=(-)^{t-j_c-j_d+1}o_2(cdt). \tag{37}$$

Similarly, matrix elements of $V_5=(Q^t\times O^t)^{(0)}$ and $V_6=(O^t\times Q^t)^{(0)}$ (the structure coefficients of Q^t and O^t are denoted as q and o) are given as follows:

$$V_5:\langle r_1\dots r_N,J_1\dots J_N|(Q^t\times O^t)^{(0)}|s_1\dots s_{N'},J_1'\dots J_{N'}'\rangle$$
$$=\delta_{NN'}\delta_{J_NJ'_{N'}}\Bigg\{\delta_{t0}\Bigg(\sum_c o(cc0)\hat{j}_c\Bigg)\langle r_1\dots r_N,J_1\dots J_N\|Q^{(0)}\|s_1\dots s_{N'},J_1'\dots J_{N'}'\rangle$$
$$+\langle r_1\dots r_N,J_1\dots J_N|(Q^t\times Q'^t)^{(0)}|s_1\dots s_{N'},J_1'\dots J_{N'}'\rangle\Bigg\},$$
$$Q'^t=\sum_{dc}q'(dct)(d^\dagger\times\tilde{c})^t,\quad q'(dct)=(-)^{t-j_c-j_d+1}o(cdt). \tag{38}$$
$$V_6:\langle r_1\dots r_N,J_1\dots J_N|(O^t\times Q^t)^{(0)}|s_1\dots s_{N'},J_1'\dots J_{N'}'\rangle$$
$$=\delta_{NN'}\delta_{J_NJ'_{N'}}\Bigg\{\delta_{t0}\Bigg(\sum_a o(aa0)\hat{j}_a\Bigg)\langle r_1\dots r_N,J_1\dots J_N\|Q^{(0)}\|s_1\dots s_{N'},J_1'\dots J_{N'}'\rangle$$
$$+\langle r_1\dots r_N,J_1\dots J_N|(Q'^t\times Q^t)^{(0)}|s_1\dots s_{N'},J_1'\dots J_{N'}'\rangle\Bigg\},$$
$$Q'^t=\sum_{ba}q'(bat)(b^\dagger\times\tilde{a})^t,\quad q'(bat)=(-)^{t-j_a-j_b+1}o(abt). \tag{39}$$

For $V_7=(\tilde{A}^t\times Q^t)^{(0)}$ and $V_8=(Q^t\times\tilde{A}^t)^{(0)}$ (the structure coefficients of $\tilde{A}^t$ and Q^t are denoted as y and q), which connect bra vectors of npnh with ket vectors of $(n+1)$p$(n+1)$h, we have formulas as below:

$$V_7\ :\ \langle r_1\cdots r_N,J_1\cdots J_N|(\tilde{A}^t\times Q^t)^{(0)}|s_1\cdots s_{N'},J_1'\cdots J_{N'}'\rangle$$
$$=\delta_{(N+1)N'}\delta_{J_NJ'_{N'}}\sum_L\frac{(2L+1)}{\hat{t}(2J_N+1)}\langle r_1\cdots r_N(t)_A,J_1\cdots J_NL\|Q^t\|s_1\cdots s_{N'},J_1'\cdots J_{N'}'\rangle, \tag{40}$$

where $(t)_A$ corresponds to $\tilde{A}^t$.

$$V_8\ :\ \langle r_1\cdots r_N,J_1\cdots J_N|(Q^t\times\tilde{A}^t)^{(0)}|s_1\cdots s_{N'},J_1'\cdots J_{N'}'\rangle$$
$$=\delta_{(N+1)N'}\delta_{J_NJ'_{N'}}\Bigg\{\sum_L\frac{(2L+1)}{\hat{t}(2J_N+1)}\langle r_1\cdots r_N(t)_A,J_1\cdots J_NL\|Q^t\|s_1\cdots s_{N'},J_1'\cdots J_{N'}'\rangle$$
$$-\langle r_1\cdots r_N(0)_{\mathcal{B}},J_1\cdots J_NJ_N|s_1\cdots s_{N'},J_1'\cdots J_{N'}'\rangle\Bigg\}, \tag{41}$$

where $(t)_A$ and $(0)_{\mathcal{B}}$ correspond to $\tilde{A}^t$ and $\tilde{\mathcal{B}}^{(0)}$, respectively. $\tilde{\mathcal{B}}^{(0)}$ is given by

$$\tilde{\mathcal{B}}^{(0)}=[\tilde{A}^t,Q^t]^{(0)}=\sum_{da}y'(da0)\tilde{A}^{(0)}(da),\quad y'(da0)=z'(da0)+(-)^{j_a+j_d+1}z'(ad0),$$
$$z'(da0)=\delta_{j_dj_a}\frac{\hat{t}}{\hat{j}_a}\sum_b(-)^{j_a+j_b+t}y(abt)q(bdt). \tag{42}$$

Similarly, matrix elements of $V_9 = (\tilde{A}^t \times O^t)^{(0)}$ and $V_{10} = (O^t \times \tilde{A}^t)^{(0)}$ (the structure coefficients of $\tilde{A}^t$ and O^t are denoted as y and o), between bra vectors of npnh and ket vectors of $(n+1)$p$(n+1)$h, are given as follows:

$$\begin{aligned} V_9 \ :\ & \langle r_1 \cdots r_N, J_1 \cdots J_N | (\tilde{A}^t \times O^t)^{(0)} | s_1 \cdots s_{N'}, J'_1 \cdots J'_{N'} \rangle \\ &= \delta_{(N+1)N'} \delta_{J_N J'_{N'}} \left\{ \delta_{t0} \left(\sum_c o(cc0) \hat{j}_c \right) \langle r_1 \cdots r_N (0)_A, J_1 \cdots J_N J_N | s_1 \cdots s_{N'}, J'_1 \cdots J'_{N'} \rangle \right. \\ &\quad \left. + \sum_L \frac{(2L+1)}{\hat{t}(2J_N+1)} \langle r_1 \cdots r_N (t)_A, J_1 \cdots J_N L \| Q^t \| s_1 \cdots s_{N'}, J'_1 \cdots J'_{N'} \rangle \right\}, \\ Q^t &= \sum_{dc} q(dct) \big(d^\dagger \times \tilde{c} \big)^t, \quad q(dct) = (-)^{t - j_c - j_d + 1} o(cdt), \end{aligned} \tag{43}$$

where $(0)_A$ and $(t)_A$ correspond to $\tilde{A}^{t=0}$ and $\tilde{A}^t$.

$$\begin{aligned} V_{10} \ :\ & \langle r_1 \cdots r_N, J_1 \cdots J_N | (O^t \times \tilde{A}^t)^{(0)} | s_1 \cdots s_{N'}, J'_1 \cdots J'_{N'} \rangle \\ &= \delta_{(N+1)N'} \delta_{J_N J'_{N'}} \left\{ \delta_{t0} \left(\sum_a o(aa0) \hat{j}_a \right) \langle r_1 \cdots r_N (0)_A, J_1 \cdots J_N J_N | s_1 \cdots s_{N'}, J'_1 \cdots J'_{N'} \rangle \right. \\ &\quad + \sum_L \frac{(2L+1)}{\hat{t}(2J_N+1)} \langle r_1 \cdots r_N (t)_A, J_1 \cdots J_N L \| Q^t \| s_1 \cdots s_{N'}, J'_1 \cdots J'_{N'} \rangle \\ &\quad \left. - \langle r_1 \cdots r_N (0)_{\mathcal{C}}, J_1 \cdots J_N J_N | s_1 \cdots s_{N'}, J'_1 \cdots J'_{N'} \rangle \right\}, \\ Q^t &= \sum_{ba} q(bat) (b^\dagger \times \tilde{a})^t, \quad q(bat) = (-)^{t - j_a - j_b + 1} o(abt), \end{aligned} \tag{44}$$

where $(0)_A$, $(t)_A$, and $(0)_{\mathcal{C}}$ correspond to $\tilde{A}^{t=0}$, $\tilde{A}^t$, and $\tilde{\mathcal{C}}^{(0)}$, respectively. $\tilde{\mathcal{C}}^{(0)}$ is given by

$$\begin{aligned} \tilde{\mathcal{C}}^{(0)} &= [\tilde{A}^t, O^t]^{(0)} = \sum_{ca} y'(ca0) \tilde{A}^{(0)}(ca), \quad y'(ca0) = z'(ca0) + (-)^{j_a + j_c + 1} z'(ac0), \\ z'(ca0) &= -\delta_{j_c j_a} \frac{\hat{t}}{\hat{j}_a} \sum_b y(abt) o(cbt). \end{aligned} \tag{45}$$

Finally, we come to $V_{11} = (\tilde{A}_1^t \times \tilde{A}_2^t)^{(0)}$:

$$\begin{aligned} V_{11} :\ & \langle r_1 \ldots r_N, J_1 \ldots J_N | \big(\tilde{A}_1^t \times \tilde{A}_2^t \big)^{(0)} | s_1 \ldots s_{N'}, J'_1 \ldots J'_{N'} \rangle \\ &= \delta_{(N+2)N'} \delta_{J_N J'_{N'}} \sum_L (-)^{J_N - L + t} \frac{\hat{L}}{\hat{J}_N \hat{t}} \big\langle r_1 \ldots r_N (t)_{A_1} (t)_{A_2}, J_1 \ldots J_N L J_N \big| s_1 \ldots s_{N'}, J'_1 \ldots J'_{N'} \big\rangle, \\ \big\langle r_1 \ldots r_N & (t)_{A_1} (t)_{A_2}, J_1 \ldots J_N L J_N M_N \big| = \langle 0 | (-)^{J_N + M_N} \Big(\big\{ [(\tilde{A}^{r_1} \times \tilde{A}^{r_2})^{(J_2)} \times \cdots \times \tilde{A}^{r_N}]^{(J_N)} \times \tilde{A}_1^t \big\}^{(L)} \times \tilde{A}_2^t \Big)^{(J_N)}_{-M_N}. \end{aligned} \tag{46}$$

D. Matrix elements for odd-number systems

The formulas in Secs. IV B and IV C remain the same for odd-number systems, except that one should replace basis states of an even-number system with those of an odd-number system. Below we exemplify this replacement by using U_4 and V_{11}:

$$\begin{aligned} U_4 :\ & \langle j r_1 \ldots r_N, J_1 \ldots J_N \| \tilde{A}^t \| j' s_1 \ldots s_{N'}, J'_1 \ldots J'_{N'} \rangle \\ &= \delta_{(N+1)N'} (-)^{J'_{N'} - J_N - t} \frac{\hat{J'}_{N'}}{\hat{J}_N} \langle j r_1 \ldots r_N (t)_A, J_1 \ldots J_N J'_{N'} | j' s_1 \ldots s_{N'}, J'_1 \ldots J'_{N'} \rangle, \\ \langle j r_1 \ldots r_N & (t)_A, J_1 \ldots J_N J'_{N'} M'_{N'} | = \langle 0 | (-)^{J'_{N'} + M'_{N'}} (\{[(\tilde{a}_j \times \tilde{A}^{r_1})^{(J_1)} \times \tilde{A}^{r_2}]^{(J_2)} \times \cdots \times \tilde{A}^{r_N}\}^{(J_N)} \times \tilde{A}^t)^{(J'_{N'})}_{-M'_{N'}}. \end{aligned} \tag{47}$$

$$V_{11}:\langle jr_1\ldots r_N,J_1\ldots J_N|\big(\tilde{A}_1^t\times\tilde{A}_2^t\big)^{(0)}|j's_1\ldots s_{N'},J_1'\ldots J_{N'}'\rangle$$
$$=\delta_{(N+2)N'}\delta_{J_NJ_{N'}'}\sum_L(-)^{J_N-L+t}\frac{\hat{L}}{\hat{J}_N\hat{t}}\big\langle jr_1\ldots r_N(t)_{A_1}(t)_{A_2},J_1\ldots J_NLJ_N\big|j's_1\ldots s_{N'},J_1'\ldots J_{N'}'\big\rangle,$$
$$\big\langle jr_1\ldots r_N(t)_{A_1}(t)_{A_2},J_1\ldots J_NLJ_NM_N\big|=\langle 0|(-)^{J_N+M_N}\big[\big(\{[(\tilde{a}_j\times\tilde{A}^{r_1})^{(J_1)}\times\tilde{A}^{r_2}]^{(J_2)}\times\cdots\times\tilde{A}^{r_N}\}^{(J_N)}\times\tilde{A}_1^t\big)^{(L)}\times\tilde{A}_2^t\big]_{-M_N}^{(J_N)}. \quad (48)$$

E. The case of doubly magic nuclei

In this subsection, we derive analytic formulas to calculate matrix elements of the SM Hamiltonian with effective interactions, for doubly magic nuclei with both proton and neutron excitations up to 2p2h. This practice not only serves as a special case of the NPA with particle-hole excitations but also is very useful in numerical calculations.

In this case, the basis states corresponding to 0p0h, 1p1h, and 2p2h excitations are in the form of $|0\rangle$, $|r_1\rangle$ (or $|s_1\rangle$) and $|r_1r_2,J_2\rangle$ (or $|s_1s_2,J_2'\rangle$), respectively. The structure coefficients of $A^{r_i\dagger}$ and $\tilde{A}^{r_i}$ (or $A^{s_i\dagger}$ and $\tilde{A}^{s_i}$) are denoted as $y(j_1j_2r_i)$ [or $y(j_1j_2s_i)$]. Nonzero matrix elements of one-body operators and two-body operators are given below in terms of overlaps with pair number $N=1$ and 2.

1. Overlap

The overlaps for basis states with $N=1$ and 2 were given in Ref. [45]. According to Eqs. (A.1) and (A.2) of Ref. [45],

$$(1)\quad \langle r_1|s_1\rangle=\delta_{r_1s_1}2\sum_{ab}y(abr_1)y(abs_1);$$

$$(2)\quad \langle r_1r_2,J_2|s_1s_2,J_2'\rangle=\delta_{J_2J_2'}\Bigg\{\delta_{r_1s_1}\delta_{r_2s_2}\Bigg[4\Bigg(\sum_{ab}y(abr_1)y(abs_1)\Bigg)\Bigg(\sum_{ab}y(abr_2)y(abs_2)\Bigg)\Bigg]$$
$$+\delta_{r_1s_2}\delta_{r_2s_1}\Bigg[4(-)^{r_1+r_2-J_2}\Bigg(\sum_{ab}y(abr_1)y(abs_2)\Bigg)\Bigg(\sum_{ab}y(abr_2)y(abs_1)\Bigg)\Bigg]$$
$$-16\hat{r}_1\hat{r}_2\hat{s}_1\hat{s}_2\sum_{a_1a_2}\sum_{b_1b_2}y(a_1a_2r_1)y(b_1b_2r_2)y(a_1b_1s_1)y(a_2b_2s_2)\begin{Bmatrix}j_{a_1}&j_{a_2}&r_1\\ j_{b_1}&j_{b_2}&r_2\\ s_1&s_2&J_2\end{Bmatrix}\Bigg\}. \quad (49)$$

Here $\begin{Bmatrix}j_{a_1}&j_{a_2}&r_1\\ j_{b_1}&j_{b_2}&r_2\\ s_1&s_2&J_2\end{Bmatrix}$ is a 9-j symbol.

2. One-body matrix elements

One-body operators include $U_1=Q^t$, $U_2=O^t$, $U_3=A^{t\dagger}$, and $U_4=\tilde{A}^t$. Based on their reduced matrix elements, one can calculate matrix elements of $H_{\pi\nu}$. For the special case of doubly magic nuclei, we have formulas as below:

$$U_1:\langle r_1\|Q^t\|s_1\rangle=(-)^{s_1-r_1+t}\frac{\hat{s}_1}{\hat{r}_1}\langle(s_1)_{\mathcal{B}}|s_1\rangle,\quad \tilde{\mathcal{B}}^{s_1}=[\tilde{A}^{r_1},Q^t]^{s_1};$$
$$\langle r_1r_2,J_2\|Q^t\|s_1s_2,J_2'\rangle=(-)^{J_2'-J_2+t}\frac{\hat{J}_2'}{\hat{J}_2}\Bigg\{\sum_{r_1'}(-)^{r_2+J_2+t+r_1'}\hat{J}_2\hat{r}_1'\begin{Bmatrix}r_1&r_2&J_2\\ J_2'&t&r_1'\end{Bmatrix}\langle(r_1')_{\mathcal{B}}r_2,J_2'|s_1s_2,J_2'\rangle$$
$$+\sum_{r_2'}(-)^{r_1+r_2+t+J_2'}\hat{J}_2\hat{r}_2'\begin{Bmatrix}r_1&r_2&J_2\\ t&J_2'&r_2'\end{Bmatrix}\langle r_1(r_2')_{\mathcal{B}},J_2'|s_1s_2,J_2'\rangle\Bigg\},$$
$$\tilde{\mathcal{B}}^{r_i'}=[\tilde{A}^{r_i},Q^t]^{r_i'},\quad i=1,2; \quad (50)$$

here $\tilde{\mathcal{B}}^{s_1}$ and $\tilde{\mathcal{B}}^{r_i'}$ can be calculated using Eq. (9).

$$U_2: \langle 0\| O^t \|0\rangle = \delta_{t0}\sum_a o(aa0)\hat{j}_a;$$

$$\langle r_1\| O^t \|s_1\rangle = \delta_{t0}\left(\sum_a o(aa0)\hat{j}_a\right)\langle r_1|s_1\rangle + (-)^{s_1-r_1+t}\frac{\hat{s}_1}{\hat{r}_1}\langle (s_1)_{\mathcal{C}}|s_1\rangle,\quad \tilde{\mathcal{C}}^{s_1} = [\tilde{A}^{r_1}, O^t]^{s_1};$$

$$\langle r_1r_2, J_2\| O^t \|s_1s_2, J_2'\rangle = \delta_{t0}\left(\sum_a o(aa0)\hat{j}_a\right)\langle r_1r_2, J_2|s_1s_2, J_2'\rangle + (-)^{J_2'-J_2+t}\frac{\hat{J}_2'}{\hat{J}_2}\left\{\sum_{r_1'}(-)^{r_2+J_2+t+r_1'}\hat{J}_2\hat{r}_1'\begin{Bmatrix} r_1 & r_2 & J_2\\ J_2' & t & r_1'\end{Bmatrix}\right.$$

$$\left.\times\langle (r_1')_{\mathcal{C}}r_2, J_2'|s_1s_2, J_2'\rangle + \sum_{r_2'}(-)^{r_1+r_2+t+J_2'}\hat{J}_2\hat{r}_2'\begin{Bmatrix} r_1 & r_2 & J_2\\ t & J_2' & r_2'\end{Bmatrix}\langle r_1(r_2')_{\mathcal{C}}, J_2'|s_1s_2, J_2'\rangle\right\},$$

$$\tilde{\mathcal{C}}^{r_i'} = [\tilde{A}^{r_i}, O^t]^{r_i'},\quad i = 1,2; \tag{51}$$

here $\tilde{\mathcal{C}}^{s_1}$ and $\tilde{\mathcal{C}}^{r_i'}$ can be calculated using Eq. (11).

$$U_3: \langle r_1\| A^{t\dagger}\|0\rangle = \delta_{r_1t}\langle r_1|(t)_A\rangle;\quad \langle r_1r_2, J_2\| A^{t\dagger}\|s_1\rangle = \langle r_1r_2, J_2|s_1(t)_A, J_2\rangle. \tag{52}$$

$$U_4: \langle 0\|\tilde{A}^t\|s_1\rangle = \delta_{s_1t}\hat{s}_1\langle (t)_A|s_1\rangle;\quad \langle r_1\|\tilde{A}^t\|s_1s_2, J_2'\rangle = (-)^{J_2'-r_1-t}\frac{\hat{J}_2'}{\hat{r}_1}\langle r_1(t)_A, J_2'|s_1s_2, J_2'\rangle. \tag{53}$$

3. Two-body matrix elements

As shown in Sec. IV C, $(A_1^{t\dagger}\times\tilde{A}_2^t)^{(0)}$ in particle representation is expressed in terms of nine operators $V_1, V_2, V_3, V_7, V_8, V_{11}, V_{12}, V_{13}, V_{14}$ [see Eq. (35) for definitions] in the mixed representation. As the Hamiltonian is Hermitian, only the up-triangle matrix elements are needed. Nonzero matrix elements for V_{12}, V_{13}, and V_{14} can be obtained from corresponding results of V_{11}, V_8, and V_7. Below we derive the matrix elements of $V_1, V_2, V_3, V_7, V_8, V_{11}$ for the case of doubly magic nuclei:

$$V_1: \langle r_1|\big(A_1^{t\dagger}\times\tilde{A}_2^t\big)^{(0)}|s_1\rangle = \delta_{r_1s_1}\delta_{r_1t}\left(\frac{2}{\hat{t}}\sum_{ab}y(abr_1)y_1(abt)\right)\big\langle (t)_{A_2}\big|s_1\big\rangle;$$

$$\langle r_1r_2, J_2|\big(A_1^{t\dagger}\times\tilde{A}_2^t\big)^{(0)}|s_1s_2, J_2'\rangle = \delta_{J_2J_2'}\left\{\delta_{r_1t}\left(\frac{2}{\hat{t}}\sum_{ab}y(abr_1)y_1(abt)\right)\big\langle (t)_{A_2}r_2, J_2\big|s_1s_2, J_2'\big\rangle\right.$$

$$+\,\delta_{r_2t}\left(\frac{2}{\hat{t}}\sum_{ab}y(abr_2)y_1(abt)\right)\big\langle r_1(t)_{A_2}, J_2\big|s_1s_2, J_2'\big\rangle$$

$$\left.+\sum_{r_1'r_2'}(-)^{r_1+r_2+J_2}\frac{\hat{r}_1'\hat{r}_2'}{\hat{t}}\begin{Bmatrix} r_1 & r_2' & r_1'\\ t & J_2 & r_2\end{Bmatrix}\big\langle (r_1')_{\mathcal{B}}(t)_{A_2}, J_2\big|s_1s_2, J_2'\big\rangle\right\},$$

$$\tilde{\mathcal{B}}^{r_1'} = \big[\tilde{A}^{r_1},\big[\tilde{A}^{r_2}, A_1^{t\dagger}\big]^{r_2'}\big]^{r_1'}; \tag{54}$$

here $\tilde{\mathcal{B}}^{r_1'}$ can be calculated using Eq. (10).

$$V_2: \langle r_1|\big(Q_1^t\times Q_2^t\big)^{(0)}|s_1\rangle = \delta_{r_1s_1}\sum_{r_1'}(-)^{r_1+t+r_1'}\frac{\hat{r}_1'}{\hat{r}_1\hat{t}}\langle (r_1)_{\mathcal{B}}|s_1\rangle,\quad \tilde{\mathcal{B}}^{r_1} = \big[\big[\tilde{A}^{r_1}, Q_1^t\big]^{r_1'}, Q_2^t\big]^{r_1};$$

$$\langle r_1r_2, J_2|\big(Q_1^t\times Q_2^t\big)^{(0)}|s_1s_2, J_2'\rangle = \delta_{J_2J_2'}\left\{\sum_{r_1'}(-)^{r_1+t+r_1'}\frac{\hat{r}_1'}{\hat{r}_1\hat{t}}\langle (r_1)_{\mathcal{B}}r_2, J_2|s_1s_2, J_2'\rangle + \sum_{r_2'}(-)^{r_2+t+r_2'}\frac{\hat{r}_2'}{\hat{r}_2\hat{t}}\langle r_1(r_2)_{\mathcal{B}}, J_2|s_1s_2, J_2'\rangle\right.$$

$$\left.+\sum_{r_1'r_2'}(-)^{r_1+t+r_2'+J_2}\frac{\hat{r}_1'\hat{r}_2'}{\hat{t}}\begin{Bmatrix} r_1 & t & r_1'\\ r_2' & J_2 & r_2\end{Bmatrix}\Big(\big\langle (r_1')_{\mathcal{B}_1}(r_2')_{\mathcal{B}_2}, J_2\big|s_1s_2, J_2'\big\rangle + \big\langle (r_1')_{\mathcal{B}_2}(r_2')_{\mathcal{B}_1}, J_2\big|s_1s_2, J_2'\big\rangle\Big)\right\},$$

$$\tilde{\mathcal{B}}^{r_i} = \big[\big[\tilde{A}^{r_i}, Q_1^t\big]^{r_i'}, Q_2^t\big]^{r_i},\quad \tilde{\mathcal{B}}_1^{r_i'} = \big[\tilde{A}^{r_i}, Q_1^t\big]^{r_i'},\quad \tilde{\mathcal{B}}_2^{r_i'} = \big[\tilde{A}^{r_i}, Q_2^t\big]^{r_i'},\quad i = 1,2; \tag{55}$$

here $\tilde{\mathcal{B}}^{r_1}$, $\tilde{\mathcal{B}}^{r_i}$, $\tilde{\mathcal{B}}_1^{r_i'}$, and $\tilde{\mathcal{B}}_2^{r_i'}$ can be calculated by (successive) applications of Eq. (9).

$$\begin{aligned}
V_3: \langle 0|\big(\tilde{A}_1^t \times A_2^{t\dagger}\big)^{(0)}|0\rangle &= 2\hat{t}\sum_{ab} y_1(abt)y_2(abt);\\
\langle r_1|\big(\tilde{A}_1^t \times A_2^{t\dagger}\big)^{(0)}|s_1\rangle &= \delta_{r_1s_1}\left\{2\hat{t}\left(\sum_{ab} y_1(abt)y_2(abt)\right)\langle r_1|s_1\rangle - \langle (r_1)_{\mathcal{B}}|s_1\rangle + \delta_{r_1t}\frac{2}{\hat{t}}\left(\sum_{ab} y(abr_1)y_2(abt)\right)\langle (t)_{A_1}|s_1\rangle\right\},\\
\tilde{\mathcal{B}}^{r_1} &= \big[\tilde{A}^{r_1},\big[\tilde{A}_1^t,A_2^{t\dagger}\big]^{(0)}\big]^{r_1};\\
\langle r_1r_2,J_2|\big(\tilde{A}_1^t \times A_2^{t\dagger}\big)^{(0)}|s_1s_2,J_2'\rangle &= \delta_{J_2J_2'}\left\{2\hat{t}\left(\sum_{ab} y_1(abt)y_2(abt)\right)\langle r_1r_2,J_2|s_1s_2,J_2'\rangle - \langle (r_1)_{\mathcal{B}}r_2,J_2|s_1s_2,J_2'\rangle - \langle r_1(r_2)_{\mathcal{B}},J_2|s_1s_2,J_2'\rangle\right.\\
&\quad + \delta_{r_1t}\left(\frac{2}{\hat{t}}\sum_{ab} y(abr_1)y_2(abt)\right)\big\langle (t)_{A_1}r_2,J_2\big|s_1s_2,J_2'\big\rangle + \delta_{r_2t}\left(\frac{2}{\hat{t}}\sum_{ab} y(abr_2)y_2(abt)\right)\\
&\quad \left.\times\big\langle r_1(t)_{A_1},J_2\big|s_1s_2,J_2'\big\rangle + \sum_{r_1'r_2'}(-)^{r_1+r_2+J_2}\frac{\hat{r}_1'\hat{r}_2'}{\hat{t}}\begin{Bmatrix} r_1 & r_2' & r_1'\\ t & J_2 & r_2\end{Bmatrix}\big\langle (r_1')_{\mathcal{B}'}(t)_{A_1},J_2\big|s_1s_2,J_2'\big\rangle\right\},\\
\tilde{\mathcal{B}}^{r_i} &= \big[\tilde{A}^{r_i},\big[\tilde{A}_1^t,A_2^{t\dagger}\big]^{(0)}\big]^{r_i},\quad i=1,2,\\
\tilde{\mathcal{B}}'^{r_1'} &= \big[\tilde{A}^{r_1},\big[\tilde{A}^{r_2},A_2^{t\dagger}\big]^{r_2'}\big]^{r_1'};
\end{aligned}\tag{56}$$

here

$$\tilde{\mathcal{B}}^{r_i} = \big[\tilde{A}^{r_i},\big[\tilde{A}_1^t,A_2^{t\dagger}\big]^{(0)}\big]^{r_i} = \sum_{a_1a_2} y'(a_1a_2r_i)(a_1^\dagger \times a_2^\dagger)^{r_i},\quad y'(a_1a_2r_i) = z'(a_1a_2r_i) - \theta(a_1a_2r_i)z'(a_2a_1r_i),$$

$$z'(a_1a_2r_i) = \frac{4\hat{t}}{2j_{a_1}+1}\sum_{b_1b_2}\delta_{j_{a_1}j_{b_2}}(-)^{r_i+t+j_{a_2}+j_{b_1}+1}y(a_2b_2r_i)y_1(a_1b_1t)y_2(b_1b_2t),$$

and $\tilde{\mathcal{B}}'^{r_1'}$ can be calculated using Eq. (10).

$$\begin{aligned}
V_7:\ \langle 0|(\tilde{A}^t \times Q^t)^{(0)}|s_1\rangle &= \delta_{s_1,0}\langle (0)_{\mathcal{B}}|s_1\rangle,\quad \tilde{\mathcal{B}}^{(0)} = [\tilde{A}^t,Q^t]^{(0)};\\
\langle r_1|(\tilde{A}^t \times Q^t)^{(0)}|s_1s_2,J_2'\rangle &= \delta_{r_1J_2'}\left\{\langle r_1(0)_{\mathcal{B}},r_1|s_1s_2,J_2'\rangle + \sum_{r_1'}(-)^{r_1+t+r_1'}\frac{\hat{r}_1'}{\hat{r}_1\hat{t}}\langle (r_1')_{\mathcal{B}'}(t)_A,r_1|s_1s_2J_2'\rangle\right\},\\
\tilde{\mathcal{B}}^{(0)} &= [\tilde{A}^t,Q^t]^{(0)},\quad \tilde{\mathcal{B}}'^{r_1'} = [\tilde{A}^{r_1},Q^t]^{r_1'};
\end{aligned}\tag{57}$$

here $\tilde{\mathcal{B}}^{(0)}$ can be calculated using Eq. (42), and $\tilde{\mathcal{B}}'^{r_1'}$ can be calculated using Eq. (9).

$$V_8: \langle r_1|(Q^t \times \tilde{A}^t)^{(0)}|s_1s_2,J_2'\rangle = \delta_{r_1J_2'}\sum_{r_1'}(-)^{r_1+t+r_1'}\frac{\hat{r}_1'}{\hat{r}_1\hat{t}}\langle (r_1')_{\mathcal{B}}(t)_A,r_1|s_1s_2,J_2'\rangle,\quad \tilde{\mathcal{B}}^{r_1'} = [\tilde{A}^{r_1},Q^t]^{r_1'};\tag{58}$$

here $\tilde{\mathcal{B}}^{r_1'}$ can be calculated using Eq. (9).

$$V_{11}: \langle 0|\big(\tilde{A}_1^t \times \tilde{A}_2^t\big)^{(0)}|s_1s_2,J_2'\rangle = \delta_{J_2',0}\big\langle (t)_{A_1}(t)_{A_2},0\big|s_1s_2,J_2'\big\rangle.\tag{59}$$

V. REALISTIC EXAMPLE OF NUMERICAL CALCULATION

In this section, we exemplify our formulation of the NPA with particle-hole excitations, by using a numerical study of the ^{100}Sn nucleus. By considering only a few collective pairs of particle-particle, hole-hole, and particle-hole types, we truncate the SM space of ^{100}Sn with both proton and neutron particle-hole excitations up to 4p4h, where valence particles are in the upper 50–82 major shell (i.e., in the $0g_{7/2},1d_{5/2},1d_{3/2},2s_{1/2},0h_{11/2}$ orbits) and valence holes in the lower 28–50 major shell (i.e., in the $0f_{5/2},1p_{3/2},1p_{1/2},0g_{9/2}$ orbits).

There have been intensive SM studies for ^{100}Sn and its neighboring nuclei; see, e.g., [68–76]. For these exotic nuclei, particle-hole excitations across closed shells are of great importance in the low-lying states. For example, for the $B(E2;0_{\rm g.s.}{}^+ \to 2_1{}^+)$ of light Sn isotopes, proton particle-hole excitations play a crucial role in the unexpected enhancement as demonstrated in Refs. [71–76], and neutron particle-hole excitations are pointed out in Ref. [76] to be important in the asymmetric feature.

The SM Hamiltonian that we use is based on the realistic low-momentum nucleon-nucleon interaction $V_{{\rm low}-k}$ [80,81,87–91]. Realistic nucleon-nucleon interactions

TABLE I. Calculated excitation energies (denoted as E_x, in unit of MeV) and $B(E2; I \to I-2)$ values (denoted as $B(E2)$ for short, in unit of W.u.), as well as the dimension of corresponding pair configuration space. Considering particles in the 50–82 major shell and holes in the 28–50 major shell, our model space with both proton and neutron particle-hole excitations up to 4p4h is constructed by using collective SD pairs of both particle-particle and hole-hole types, as well as collective positive-parity particle-hole pairs with spin 2, 4, and 6, respectively. The unscreened effective charges, i.e., $e_\pi = 1.5e$ and $e_\nu = 0.5e$, are adopted to calculated $B(E2)$ values.

	Dimension	E_x [MeV]	$B(E2)$ [W.u.]
0_1^+	4211	0	
2_1^+	17619	5.34	8.52
4_1^+	23486	5.85	0.54
6_1^+	21225	6.07	0.48

[78–82] have been very successful as microscopic input of nuclear many-body problems. In particular, the low-momentum interaction [80,81,87–91] has the remarkable feature that renormalized $V_{\text{low}-k}$ interactions from various free-space NN potentials all flow to an unique one. The $V_{\text{low}-k}$ matrix elements used here [92] are derived from the CD-Bonn potential [93], with the decimation momentum $\Lambda = 2.0\ \text{fm}^{-1}$. The harmonic oscillator parameter $\hbar\omega$ is taken to be 8.5 MeV, given by the widely used formula $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ [94].

For the two-body interaction, $V_{JT}(j_1 j_2 j_3 j_4)$ of Eq. (26) is taken to be $\langle j_1 j_2 JT | V_{\text{low}-k} | j_3 j_4 JT\rangle$. For the single-particle energies with respect to the frozen ^{56}Ni core (denoted as ε_j), together with monopoles of the $V_{\text{low}-k}$ matrix elements, they are fixed to reproduce the single-particle energies with respect to ^{100}Sn (denoted as ε'_j) summarized in Ref. [95]:

$$\varepsilon'_j = \varepsilon_j + \frac{1}{2(2j+1)} \sum_{j_\text{h}} \left(1 + \delta_{j j_\text{h}}\right) \sum_{JT} (2J+1)(2T+1) \times \langle j_\text{h} j JT | V_{\text{low}-k} | j_\text{h} j JT \rangle, \tag{60}$$

where j_h labels an orbit in the lower 28–50 major shell. The single-particle energies summarized in Ref. [95] indicate the $Z = 50$ and $N = 50$ shell gaps in ^{100}Sn are 5.96 and 6.35 MeV, respectively.

We use the method of Ref. [96] to eliminate the spurious center-of-mass motion, i.e., adopt the Hamiltonian in the particle representation as follows:

$$H = H_\text{SM} + \beta\left(H_\text{CM} - \frac{3}{2}\hbar\omega\right), \quad H_\text{CM} = \frac{\tilde{P}^2}{2mA} + \frac{1}{2} m A \omega^2 \tilde{R}^2. \tag{61}$$

Here H_SM is the SM Hamiltonian, A is the mass number of the calculated nucleus, and $\tilde{P}$ and $\tilde{R}$ are the center-of-mass momentum and coordinate, respectively. In our calculation, $\beta\hbar\omega/A$ for ^{100}Sn is set to be 10 MeV.

In our calculation, we adopt collective SD pairs of both particle-particle and hole-hole types, as well as collective positive-parity particle-hole pairs with spin 2, 4, and 6, respectively. The structure coefficients are obtained directly from corresponding two-body wave functions. For both proton part and neutron part, the maximum number of particle-hole pairs coupled in a basis state is limited to be one. In Table I, we present the dimensions for $0^+, 2^+, 4^+, 6^+$ in our model space. One sees our dimensions are drastically smaller than corresponding ones in the J-scheme shell model, which are at the order of 10^{13}. In Table I, we also present the calculated excitation energies and $B(E2; I \to I-2)$ values for the $2_1^+, 4_1^+, 6_1^+$ states. The unscreened effective charges, i.e., $e_\pi = 1.5e$ and $e_\nu = 0.5e$, are adopted in this study. Our results are close to the SM ones summarized in Ref. [95], which are calculated considering less single-j orbits.

VI. SUMMARY

In this paper, we develop the formalism for the nucleon-pair approximation (NPA) with particle-hole excitations, in which particles and holes are treated simultaneously. By using this approach, one is able to perform multiple-major-shell NPA calculations. Technically, we use a mixed representation, i.e., the particle-hole conjugate transformation is used for operators of the lower major shells, while operators of the upper major shells remain unchanged. Therefore, three types of nucleon pairs, i.e., valence-particle pairs in the upper major shells, valence-hole pairs in the lower major shells, and pairs consisting of one valence particle in the upper shells and one valence hole in the lower ones, are treated on the same footing.

We construct basis states by coupling collective pairs of the above three types. The SM Hamiltonian (with either effective interactions or phenomenological pairing plus multipole-multipole interactions) are transformed correspondingly in the mixed representation, and we derive formulas to calculate matrix elements of one- and two-body operators. As a special case, for doubly magic nuclei with both proton and neutron excitations up to 2p2h, we present analytical formulas for matrix elements of the SM Hamiltonian with effective interactions.

To exemplify our approach, we calculate ^{100}Sn considering both proton and neutron particle-hole excitations up to 4p4h, where valence particles are in the upper 50–82 major shell and valence holes in the lower 28–50 major shell, with the low-momentum nucleon-nucleon interaction derived from the CD-Bonn potential. Because the NPA uses collective pairs and thus has an advantage on the issues involving many active single-j orbits, we believe the approach of this work will be very useful in microscopic studies of exotic nuclei and nuclear shape coexistence in middle-heavy and heavy regions.

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