Generalized quantization formalism

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(Received 17 August 1990)

A generalized quantization formalism (QF) is proposed which works for the partial space (e.g., the orbital, or spin, or color) space as well as for the total space. The creation and annihilation operators in the generalized QF are in general neither boson nor fermion operators. However, if we restrict ourselves to the totally antisymmetric (symmetric) states (including any intermediate states), then they are reduced to the fermion (boson) operators. Therefore, the generalized QF is an extension of the second QF. The generalized QF is superior to both the first and second QF for computing the matrix elements in a basis which has definite symmetry in each subspace. Using the generalized QF, the shell-model calculation for the multishell, multispin case is reduced to that for the single-shell, single-spin case, and the Brussaard and Glaudemans results become the trivial case of two shell and zero spin, i.e., the case $(\gamma_1^{n_1}\gamma_2^{n_2})$, where $\gamma=j$ or jt.

I. INTRODUCTION

In nuclear physics or particle physics we often need to deal with multishell and multispin cases. For example, in nuclear physics we need to calculate the matrix elements of $[C^\dagger_{j_\alpha t}\times C_{j_\beta t}]^{JT}$, where $C^\dagger_{jm_jtm_t}$ are creation operators in the second quantized form, and $\alpha,\beta=1,2\ldots$, while in particle physics, the matrix elements of $[C^\dagger_{l_\alpha cfs}\times C_{l_\beta cfs}]^{L(\lambda_c\mu_c)(\lambda_f\mu_f)S}$, etc., where c, f, and s are indices for the color, flavor, and spin, respectively, and $(\lambda_c\mu_c),(\lambda_f\mu_f)$ are SU(3) irreducible representation (irrep) labels. The labor involved in the calculation increases drastically with the increase of the number of shells and spins involved. Several schemes of calculation for the two-shell case have been proposed.[1–5] All these schemes are not very practical and have not been programmed due to their complexity. The available multishell shell-model codes are based either on the *j-j* coupling scheme or the *m* scheme.[6] The former is based on the scheme of first antisymmetrizing each single (jt) space and then antisymmetrizing the total space, i.e., using the basis $|[1^n]$: $(j_1t)^{n_1}[1^{n_1}],(j_2t)^{n_2}[1^{n_2}],\ldots)$ with $n=n_1+n_2+\cdots$. The Oak Ridge code[7] and Ritsschil code[8] belong to this scheme. Tutorial monographs on this approach are available.[9,10]

Recently a powerful new approach[11] to the two-shell and two-spin problem is proposed with the following coupling scheme: $|[1^n]$: $((j_1)^{n_1}[\nu_1],(j_2)^{n_2}[\nu_2])[\nu]$; $(t)^n[\tilde{\nu}])$, which is based on the assumption that the creation and annihilation operators, $C^\dagger_{jm_jtm_t},C_{jm_jtm_t}$, can be factored into products of operators acting in the separate subspace,[12,13]

$$C^\dagger_{jm_jtm_t}=C^\dagger_{jm_j}C^\dagger_{tm_t}\,,\quad C_{jm_jtm_t}=C_{jm_j}C_{tm_t}\,. \tag{1}$$

The matrix elements of one-body and two-body operators are likewise factored into a product of the matrix elements for each individual subspace and the coupling coefficients between the different subspaces. Since the dimensions of the factored subspaces are generally much smaller than the dimension of the space carrying the antisymmetric fermion wave functions, the calculation can be extended into regions beyond the feasibility limits of modern shell-model codes. A code DUSM (Drexel University shell model) based on the factorization is currently under development.

Although the factorization (1) greatly simplifies the calculation of the matrix elements, the interpretation of (1) as the factorization of second quantized operators is not correct. As we know that the second quantization formalism (QF) applies only to the total space where particles are indistinguishable and thus are not labeled by particle indices. In the partial space where particles are distinguishable, we need to use the first QF where both states and operators have particle indices. The operators $C^\dagger_{jm_j},C^\dagger_{tm_t}$, etc., for partial spaces in (1) have no particle indices and are meaningless. In other words, *the second quantized operator cannot be factored.* Besides, in Ref. 11 only the main idea behind the algorithm is outlined without neither going to the detail of derivation nor providing explicitly all the essential formulas. The formalism in Ref. 11 is rather cumbersome and is hard to be generalized to the multishell, multispin cases.

In this paper we are going to introduce a generalized QF, where the states have particle labels and the operators have implicit particle labels. The generalized QF can be applied to both the partial space and total space. The creation (annihilation) operator $a^\dagger_\alpha$ (a_α) in the generalized QF is in general neither a boson nor fermion operator, and is called a hybrid operator. It is the hybrid operator which is factorizable. If we restrict ourselves to the totally antisymmetric (symmetric) states (including any intermediate states), then it is reduced to the fermion (boson) operator. In this sense the generalized QF is an extension of the second QF. The present paper is organized as follows. In Sec. II, the generalized creation and annihilation operators are defined, whose reduced matrix elements are related to the reduced Wigner coefficients, or coefficients of fractional parentage (CFP). In Sec. III, the relation between the matrix elements in the generalized and second QF are discussed. In Sec. IV, the matrix elements for the one- and two-body operators are cast into a form which allows us to generalize it to a multishell, multispin case in a straightforward way. In Sec. V the multishell, multispin case is treated in detail. Finally, Sec. VI contains a comparison among the three QF.

II. THE GENERALIZED CREATION AND ANNIHILATION OPERATORS AND THEIR FACTORIZATION

In the following the first, second, and generalized operators are denoted by the following:

First QF, $a_\alpha^\dagger(i)\ [a_\alpha(i)]$;

second QF, $C_\alpha^\dagger(C_\alpha)$;

generalized QF, $a_\alpha^\dagger\ (a_\alpha)$;

where $\alpha,\beta,\ldots$ are state labels and $i,j,\ldots$ are particle labels. The operators $a_\alpha^\dagger$ and a_α are to be defined.

Suppose that in a certain space, which could be a partial space, such as orbital space, spin space, or a total space, we have a set of single-particle (s.p.) states $\alpha,\beta,\gamma,\ldots$, which carry the fundamental representation of the unitary group SU(N).

Definition 1. The creation (annihilation) operator $a_\alpha^\dagger$ (a_α), called the hybrid operator, in the generalized QF creates (annihilates) the *last* particle in the state α,

$$\begin{aligned} a_\alpha^\dagger|\Psi(1,2,\ldots,n)\rangle &= |\Psi(1,2,\ldots,n)\rangle|\psi_\alpha(n+1)\rangle\ , \\ a_\alpha|\Psi(1,2,\ldots,n-1)\psi_\beta(n)\rangle &= \delta_{\alpha\beta}|\Psi(1,2,\ldots,n-1)\rangle\ . \end{aligned} \tag{2}$$

Suppose that $\Psi(1,2,\ldots,n)$ is the Yamanouchi basis $|[\nu]\mu\rangle$ of the permutation group S_n and an irreducible basis $|[\nu]w\rangle$ of SU(N), denoted by $|[\nu]\mu,w\rangle$, where $[\nu]$ is the partition, w any convenient subgroup labels of the unitary group, and μ the Yamanouchi symbol $(r_{n-1},r_{n-2},\ldots,r_1)$. By inserting a complete set of intermediate states, we have

$$a_\alpha^\dagger|[\nu]\mu,w\rangle = \sum_{\nu^0\mu^0w^0}|[\nu^0]\mu^0,w^0\rangle \times\langle[\nu^0]\mu^0,w^0|a_\alpha^\dagger|[\nu]\mu,w\rangle\ . \tag{3}$$

In this paper we often use ν^{00}, ν^0, ν, ν', and ν'' to denote the irrep labels for the states with $n+2$, $n+1$, n, $n-1$, and $n-2$ particles, respectively, and similarly for other quantum numbers, e.g., μ,w, etc. Notice that due to the branching rule of the permutation group we have $[\nu^0]\mu^0=[\nu^0][\nu]\mu=[\nu^0][\nu][\nu']\mu',\ldots$. Since $a_\alpha^\dagger$ is the creation operator for the $(n+1)$th particle, it is a scalar of S_n. Therefore it will not change the quantum number ν and its matrix elements are independent of μ,

$$\begin{aligned}\langle[\nu^0]\mu^0,w^0|a_\alpha^\dagger|[\nu]\mu,w\rangle &= \langle[\nu^0]\nu,w^0|a_\alpha^\dagger|[\nu]w\rangle \\ &= \langle[\nu^0]w^0|a_\alpha^\dagger|[\nu]w\rangle\ ,\end{aligned} \tag{4}$$

where in the right-hand side we delete the quantum number ν in the bra vector $\langle[\nu^0]\nu w^0|$, since it has to be the same as in the ket vector $|[\nu]w\rangle$. Keeping only the essential quantum numbers, Eq. (3) can be rewritten as

$$a_\alpha^\dagger|[\nu],w\rangle = \sum_{\nu^0w^0}|[\nu^0]\nu,w^0\rangle\langle[\nu^0]\nu,w^0|a_\alpha^\dagger|[\nu]w\rangle\ . \tag{5}$$

It is easy to identify the matrix element of the hybrid operator with the SU(N) Clebsch-Gordan coefficients $\langle[\nu^0]w^0|[\nu]w,[1]\alpha\rangle$,

$$\langle[\nu^0]w^0|a_\alpha^\dagger|[\nu]w\rangle = \langle[\nu^0]w^0|[\nu]w,[1]\alpha\rangle\ . \tag{6}$$

The operator $a_\alpha^\dagger$ (a_α) can be visualized as the operation of adding (removing) one box to (from) the Young diagram $[\nu]$.

Suppose that G is a subgroup of U(N), then the G-reduced matrix element (in the definition of Ref. 14) of a hybrid operator is the U(N)$\supset G$ isoscalar factors (ISF),

$$\langle[\nu]\alpha\Lambda\|a_\lambda^\dagger\|[\nu']\alpha'\Lambda'\rangle = \langle[\nu]\alpha\Lambda\|[\nu']\alpha'\Lambda',[1]\lambda\rangle\ , \tag{7}$$

where Λ is the irrep label of the subgroup G, and α is the inner multiplicity label (not to be confused with the single-particle state label) for the subduction $[\nu]\downarrow\Lambda$.

Specifying to the orbital space, the SO(3) reduced matrix element of the hybrid operator $a_l^\dagger$ in the SU($2l+1$)$\supset$SO(3) basis is the SU($2l+1$)$\supset$SO(3) ISF,[5] or the one-body orbital CFP,

$$\langle[\nu^0]\alpha^0L^0\|a_l^\dagger\|[\nu]\alpha L\rangle = \langle l^{n+1}[\nu^0]\alpha^0L^0\{|l^n[\nu]\alpha L,l\rangle\ . \tag{8}$$

The definition (8) for the matrix elements of the hybrid operator $a_l^\dagger$ differs from Eq. (5) of Ref. 13 and Eq. (2.5) of Ref. 11 by a factor $[n(2L^0+1)]^{1/2}$.

Notice that in Eq. (5) the irrep label ν^0 for the intermediate states is a summation index. For example, if $[\nu]=[1^n]$, then $[\nu^0]$ has two possible values, $[1^{n+1}]$ and $[21^{n-1}]$. In the following we often use the phrase "restricting to totally antisymmetric (symmetric) states" or "in totally antisymmetric (symmetric) spaces." It means that all the initial, final, and intermediate states are totally antisymmetric (symmetric). To implement such a restriction it is convenient to introduce the operator $\hat{a}^\dagger$ which is equal to the product of the antisymmetrizer $P^{[1^{n+1}]}$ (or symmetrizer $P^{[n+1]}$) with the hybrid operator $a_\alpha^\dagger$,

$$\begin{aligned}\hat{a}_\alpha^\dagger &= P^{[1^{n+1}]}a_\alpha^\dagger\ , \\ \hat{a}_\alpha^\dagger|[1^n]w\rangle &= \sum_{w^0}|[1^{n+1}]w^0\rangle\langle[1^{n+1}]w^0|a_\alpha^\dagger|[1^n]w\rangle\ .\end{aligned} \tag{9}$$

Up to now there is nothing new. Essentially we are still within the first QF. One can say that we merely simplified the notation: replacing $a_\alpha^\dagger(n+1)$ and $a_\alpha(n)$ by $a_\alpha^\dagger$ and a_α, respectively. The difference between the first and generalized QF's arises as soon as the pair-creation operator is involved. According to our Definition 1

$$\begin{aligned} a_\alpha^\dagger a_\beta^\dagger&|\Psi(1,2,\ldots,n-2)\rangle \\ &= |\Psi(1,2,\ldots,n-2)\psi_\beta(n-1)\psi_\alpha(n)\rangle\ , \end{aligned} \tag{10}$$

$$a_\beta^\dagger a_\alpha^\dagger|\Psi(1,2,\ldots,n-2)\rangle = |\Psi(1,2,\ldots,n-2)\psi_\alpha(n-1)\psi_\beta(n)\rangle \ . \quad (11)$$

Therefore, $a_\alpha^\dagger$ and $a_\beta^\dagger$ neither commute nor anticommute. Similarly for a_α and a_β,

$$[a_\alpha^\dagger,a_\beta^\dagger]_\pm \neq 0, \quad [a_\alpha,a_\beta]_\pm \neq 0 \ , \quad (12)$$

in contrast to the first QF and second QF,

$$[a_\alpha^\dagger(i),a_\beta^\dagger(j)]=0 \ \text{ for fermion or boson} \ ,$$

$$[C_\alpha^\dagger,c_\beta^\dagger]_\pm=0 \ \text{ for } \begin{cases}\text{fermion}\\ \text{boson}\end{cases} .$$

From Definition 1, it is obvious that

$$a_\alpha a_\beta^\dagger \equiv \delta_{\alpha\beta} \ . \quad (13)$$

However, in general, $a_\beta^\dagger a_\alpha \neq 0$, even $\alpha\neq\beta$; $a_\beta^\dagger a_\alpha$ shifts the last particle from the state α to the state β. Equation (13) shows that $a_\alpha a_\beta^\dagger$ is a c number and we have

$$\langle \bar{\nu}\bar{\Gamma}\| a_{jm'}a_{jm}^\dagger \|\nu\Gamma\rangle = \delta_{\bar{\nu}\nu}\delta_{\bar{\Gamma}\Gamma}\delta_{m'm} \ , \quad (14)$$

where $\Gamma\equiv JM$. It is thus seen that the order of the operators in the generalized QF is crucial. We never change the order of the operators for the same shell in computing the matrix elements of one- or two-body operators. In the actual calculation, we only use the normal-ordered operators such as $a_\alpha^\dagger a_\beta$, $a_\alpha^\dagger a_\beta^\dagger$, $a_\alpha a_\beta$, $a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta$, etc., and never use the non-normal-ordered operators such as $a_\alpha a_\beta^\dagger$.

An essential difference between the normal order and non-normal order hybrid operators is that in calculating the matrix elements of the former between two totally antisymmetric (symmetric) states, all the intermediate states are necessarily totally antisymmetric (symmetric), while for the latter the intermediate states may include other states; see Eq. (18) given below.

Since the hybrid operators $a_{jm_jtm_t}^\dagger$ ($a_{jm_jtm_t}$) are creation operators for a specific (the last) particle, they are factorizable

$$a_{jm_jtm_t}^\dagger = a_{jm_j}^\dagger a_{tm_t}^\dagger, \quad a_{jm_jtm_t}=a_{jm_j}a_{tm_t} \ . \quad (15a)$$

The factorization of (15a) is recursive and can be applied to any combined space, for example,

$$a_{lcfs}^\dagger = a_l^\dagger a_{cfs}^\dagger = a_l^\dagger a_c^\dagger a_{fs}^\dagger = a_l^\dagger a_c^\dagger a_f^\dagger a_s^\dagger \ . \quad (15b)$$

Obviously, the hybrid operators acting on different subspaces commute. These properties enable us to "factorize" (summing over intermediate quantum numbers) the matrix elements of any product of the hybrid operators; see Eqs. (22)–(27) given below.

III. THE HYBRID OPERATOR IN THE TOTALLY ANTISYMMETRIC OR SYMMETRIC SPACE

Now let us use $\alpha,\beta,\ldots,$ to denote the single-particle state in the totally antisymmetric (or symmetric) space. It could be $lm_l, jm_j, jm_jtm_t, lm_lsm_s$, etc. According to the well-known fact that the matrix element of a one-body operator between two totally symmetric (or antisymmetric) n-particle states is equal to n times that of the one-body operator referring to a specific, say, the nth particle, we have

$$([n]w|C_\alpha^\dagger C_\beta|[n]w) = n([n]w|a_\alpha^\dagger a_\beta|[n]w) \ . \quad (16)$$

From (16) and (9) we obtain the relation between the second and generalized QF,

$$C_\alpha^\dagger|[n]w) = \sqrt{n+1}\,\hat{a}_\alpha^\dagger|[n]w) \ , \qquad C_\alpha|[n]w) = \sqrt{n}\,a_\alpha|[n]w) \ . \quad (17)$$

From (17) we immediately obtain the relation between the matrix elements of the operators in the second QF and the generalized QF,

$$\begin{aligned}
&([n]w|C_\alpha^\dagger|[n-1]w') = \sqrt{n}\,([n]w|a_\alpha^\dagger|[n-1]w') \ , \\
&([n]|C_\beta C_\alpha^\dagger[n]) = (n+1)([n]|a_\beta\hat{a}_\alpha^\dagger|[n]) \ , \\
&([n]|C_\alpha^\dagger C_\beta^\dagger|[n-2]) = \sqrt{n(n-1)}([n]|a_\alpha^\dagger a_\beta^\dagger|[n-2]) \ , \\
&([n]|C_\alpha^\dagger C_\beta^\dagger C_\gamma c_\delta|[n]) = n(n-1)([n]|a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta|[n]) \ , \\
&([n]|C_\alpha^\dagger C_\beta^\dagger C_\gamma|[n-1]) \\
&\qquad = (n-1)\sqrt{n}\,([n]|a_\alpha^\dagger a_\beta^\dagger a_\gamma|[n-1]) \ , \\
&([n]|C_\alpha^\dagger C_\gamma C_\delta|[n+1]) = n\sqrt{n+1}([n]|a_\alpha^\dagger a_\gamma a_\delta|[n+1]) \ .
\end{aligned} \quad (18)$$

For the totally antisymmetric states, we have the same results.

From (18) we know that in the totally antisymmetric space, $a_\alpha^\dagger$ and $a_\beta^\dagger$ anticommute,

$$\{a_\alpha^\dagger,a_\beta^\dagger\}=0 \ , \quad (19a)$$

while in the totally symmetric space $a_\alpha^\dagger$ and $a_\beta^\dagger$ commute,

$$[a_\alpha^\dagger,a_\beta^\dagger]=0 \ . \quad (19b)$$

Letting $\alpha=jm$, from $\{C_{jm_1},C_{jm_2}^\dagger\}=\delta_{m_1m_2}$ and (17) we have

$$(n+1)a_{jm_1}\hat{a}_{jm_2}^\dagger + n\hat{a}_{jm_2}^\dagger a_{jm_1} = \delta_{m_1m_2} \ , \quad (20)$$

when it is acting on the state $|[1^n])$. Notice that if there is no restriction on the intermediate states we would have $a_{jm_1}a_{jm_2}^\dagger = \delta_{m_1m_2}$.

From Eqs. (18)–(20) we conclude that in the totally antisymmetric space, the generalized operators (apart from nonessential factors) reduce to the fermion operators. Similarly, in the totally symmetric space, they reduce to the boson operators.

IV. APPLICATION TO THE SINGLE-SHELL AND SINGLE-SPIN CASES

We will use parentheses to denote a totally antisymmetric state, while the angular brackets denote a state with arbitrary symmetry. For convenience in exposition, we use l and s to denote *two arbitrary* unitary quantum numbers, which does not mean that we deal with the L-S coupling only, since l and s could be j and t. A totally antisymmetric state is classified according to the irrep labels of the following group chain:

$$\begin{matrix} \mathrm{U}(MN) \supset (\mathrm{U}(M) \supset \mathrm{SO}(3)) \times (\mathrm{U}(N) \supset \mathrm{SU}(2)) \\ [1^n] \quad [\nu] \quad \alpha L M_L \quad [\tilde{\nu}] \quad \beta S M_S \end{matrix} , \tag{21}$$

where M (N) is the total number of the s.p. states in the l (s) subspace, $[\nu]$ is the partition of n, while β is the multiplicity label for the reduction $\mathrm{U}(N)\downarrow\mathrm{SU}(2)$. The orbital, spin, and total spaces will be termed as the spaces V^M, V^N, and V^{MN}, respectively, $V^{MN}=V^M\otimes V^N$.

A. Single-particle creation operator

The isoscalar factor corresponding to the group chain (21) is the total CFP and can be factorized [see Eq. (7-185) in Ref. 5],

$$\begin{aligned}([1^n][\nu]\alpha L,\beta S\|a_{ls}^\dagger\|[1^{n-1}][\nu']\alpha' L',\beta' S') &= (\nu|b^\dagger|\nu')\langle[\nu]\alpha L\|a_l^\dagger\|[\nu']\alpha' L'\rangle \\ &\times\langle[\tilde{\nu}]\beta S\|a_s^\dagger\|[\tilde{\nu}']\beta' S'\rangle ,\end{aligned} \tag{22a}$$

where $(\nu|b^\dagger|\nu')$ is the $\mathrm{U}(MN)\supset\mathrm{U}(M)\times\mathrm{U}(N)$ ISF,[15]

$$\begin{aligned}(\nu|b^\dagger|\nu')=(\nu'|b|\nu)&\equiv(\nu\tilde{\nu},[1^n]|b^\dagger|\nu'\tilde{\nu}',[1^{n-1}]) \\ &=\Lambda_{\nu'}^{\nu}\sqrt{h_{\nu'}/h_\nu} ,\end{aligned} \tag{22b}$$

where h_ν is the dimension of the irrep ν of the permutation group S_n, $\Lambda_{\nu'}^{\nu}$ is the relative phase factor for the Yamanouchi basis first introduced by Butler,[16] and $[\tilde{\nu}]$ is the conjugation of the partition $[\nu]$. The creation operator $b^\dagger$ can be visualized as the operation of adding one box to both the orbital and spin Young diagrams $[\nu']$ and $[\tilde{\nu}']$. Notice the difference between the creation operator $a_l^\dagger$ ($a_s^\dagger$) in the orbital space V^M (spin space V^N), and the creation operator $b^\dagger$, the former adds one box only to the Young diagram $[\nu']$ ($[\tilde{\nu}']$).

If s is the usual spin, then $\langle[\tilde{\nu}]\beta S\|a_s^\dagger\|[\tilde{\nu}']\beta' S'\rangle$ is the single-particle CFP in the spin space. The space spanned by the basis $|\nu)\equiv|\nu\tilde{\nu},[1^n])$ will be denoted by $\mathbb{V}^{MN}$

$$\mathbb{V}^{MN}=\{|\nu): [\nu]\in \text{ any partitions of the integer } n\} , \tag{22c}$$

with dimension equal to the number of partitions of the integer n.

By inserting a complete set of intermediate states between two operators and using (22a), we can generalize the factorization (22a) for a single creation operator to any product of the creation and annihilation operators. Several examples are given below.

B. Pair-creation operator

$$([1^n][\nu]\alpha L,\beta S\|[a_{ls}^\dagger\times a_{ls}^\dagger]^{kq}\|[1^{n-2}][\nu'']\alpha'' L'',\beta'' S'') =\sum_{\nu'}(\nu|b^\dagger b^\dagger|\nu'')_{\nu'}\langle[\nu]\alpha L\|[a_l^\dagger\times a_l^\dagger]^k\|[\nu'']\alpha'' L''\rangle^{\nu'}\langle[\tilde{\nu}]\beta S\|[a_s^\dagger\times a_s^\dagger]^q\|[\tilde{\nu}'']\beta'' S''\rangle^{\tilde{\nu}'} . \tag{23a}$$

The $\mathrm{U}(MN)\supset\mathrm{U}(M)\times\mathrm{U}(N)$ two-body ISF $(\nu|b^\dagger b^\dagger|\nu'')_{\nu'}$ can be factorized,

$$(\nu|b^\dagger b^\dagger|\nu'')_{\nu'}=(\nu|b^\dagger|\nu')(\nu'|b^\dagger|\nu'')=\Lambda_{\nu'}^{\nu}\Lambda_{\nu''}^{\nu'}\sqrt{h_{\nu''}/h_\nu} . \tag{23b}$$

C. One-body operator

$$([1^n][\bar{\nu}]\bar{\alpha}\bar{L},\bar{\beta}\bar{S}\|[a_{ls}^\dagger\times\tilde{a}_{ls}]^{kq}\|[1^n][\nu]\alpha L,\beta S)=\sum_{\nu'}(\bar{\nu}|b^\dagger b|\nu)_{\nu'}\langle[\bar{\nu}]\bar{\alpha}\bar{L}\|[a_l^\dagger\times\tilde{a}_l]^k\|[\nu]\alpha L\rangle^{\nu'}\langle[\tilde{\bar{\nu}}]\bar{\beta}\bar{S}\|[a_s^\dagger\times\tilde{a}_s]^q\|[\tilde{\nu}]\beta S\rangle^{\tilde{\nu}'} , \tag{24a}$$

$$(\bar{\nu}|b^\dagger b|\nu)_{\nu'}=(\bar{\nu}|b^\dagger|\nu')(\nu'|b|\nu)=\Lambda_{\nu'}^{\bar{\nu}}\Lambda_{\nu'}^{\nu}\frac{h_{\nu'}}{\sqrt{h_{\bar{\nu}}h_\nu}} . \tag{24b}$$

For later convenience, $(\bar{\nu}|b^\dagger b|\nu)_{\nu'}$ will be referred to as the one-body matrix elements in the space $\mathbb{V}^{MN}$ defined by (22c). Notice that (1) the one-body operator $[a_l^\dagger\times\tilde{a}_l]^k$ is a scalar of S_{n-1} with its matrix elements being diagonal in $\nu'\mu'$ and independent of the component index μ'; (2) the representative matrix of $[a_l^\dagger\times\tilde{a}_l]^k$ is not diagonal in ν, since $[a_l^\dagger\times\tilde{a}_l]^k$ is not a generator of the unitary group $\mathrm{U}(2l+1)$ [in fact, it is a generator of the group $\mathrm{U}^{(n)}(2l+1)$ acting only on the nth particle].

The matrix elements

$$\langle[\nu]\alpha L\|[a_l^\dagger\times a_l^\dagger]^k\|[\nu'']\alpha'' L''\rangle^{\nu'},\quad \langle[\bar{\nu}]\bar{\alpha}\bar{L}\|[a_l^\dagger\times\tilde{a}_l]^k\|[\nu]\alpha L\rangle^{\nu'},\quad\text{and}\quad \langle[\nu'']\alpha'' L''\|[\tilde{a}_l\times\tilde{a}_l]^k\|[\nu]\alpha L\rangle^{\nu'} ,$$

as well as the corresponding matrix elements in the spin space, can be calculated by

$$\langle[\bar{\nu}]\bar{\alpha}\bar{L}\|Y_{k_1}\times Z_{k_2}]^k\|[\nu]\alpha L\rangle^{\nu'}=\sum_{\alpha' L'}(-)^{k_1+k_2-k}U(Lk_2\bar{L}k_1;L'k)\langle[\bar{\nu}]\bar{\alpha}\bar{L}\|Y_{k_1}\|[\nu']\alpha' L'\rangle\langle[\nu']\alpha' L'\|Z_{k_2}\|[\nu]\alpha L\rangle , \tag{24c}$$

where Y_{k_1} and Z_{k_2} are irreducible tensors of ranks k_1 and k_2, respectively.

As an example, using (18), (24), and the fact that the CFP

$$\langle[2]L\|a_l^\dagger\|[1]l\rangle=\langle[11]S\|a_s^\dagger\|[1]s\rangle=1 , \tag{25a}$$

we immediately get the following one-body matrix element,

$$([1^2][2]\bar{L}\bar{S}\|[C_{ls}^{\dagger}\times\tilde{C}_{ls}]^{kq}\|[1^n][2]LS)=2(-)^{L-k+S-q}\left[\frac{(2L+1)(2S+1)}{(2l+1)(2s+1)}\right]^{1/2}U(Ll\bar{L}l;lk)U(Ss\bar{S}s;sq)\ . \tag{25b}$$

D. Two-body operator: $V(kq)=[a_{ls}^{\dagger}\times a_{ls}^{\dagger}]^{kq}\cdot[\tilde{a}_{ls}\times\tilde{a}_{ls}]^{kq}$

The scalar product of two tensors is defined by

$$U^k\cdot V^k=\sqrt{2k+1}[U^k\cdot V^k]_0^0\ .$$

By introducing the two-body generalized operators in the orbital and spin spaces,

$$V(k)=[a_l^{\dagger}\times a_l^{\dagger}]^k\cdot[\tilde{a}_l\times\tilde{a}_l]^k,\quad V(q)=[a_s^{\dagger}\times a_s^{\dagger}]^q\cdot[\tilde{a}_s\times\tilde{a}_s]^q\ ,$$

the two-body matrix element can be expressed as

$$([1^n][\bar{\nu}]\bar{\alpha}L,\bar{\beta}S\|V(kq)\|[1^n][\nu]\alpha L,\beta S)=\sum_{\bar{\nu}'\nu''\nu'}(\bar{\nu}|b^{\dagger}b^{\dagger}bb|\nu)_{\bar{\nu}'\nu''\nu'}\langle[\bar{\nu}]\bar{\alpha}L\|V(k)\|[\nu]\alpha L\rangle^{\bar{\nu}'\nu''\nu'}\langle[\tilde{\bar{\nu}}]\bar{\beta}S\|V(q)\|[\tilde{\nu}]\beta S\rangle^{\tilde{\bar{\nu}}'\tilde{\nu}''\tilde{\nu}'}\ . \tag{26a}$$

The matrix element $(\bar{\nu}|b^{\dagger}b^{\dagger}bb|\nu)_{\bar{\nu}'\nu''\nu'}$ will be called the two-body matrix element in the space $\mathbb{V}^{MN}$ and can be factorized

$$(\bar{\nu}|b^{\dagger}b^{\dagger}bb|\nu)_{\bar{\nu}'\nu''\nu'}=(\bar{\nu}|b^{\dagger}b^{\dagger}|\nu'')_{\bar{\nu}'}(\nu''|bb|\nu)_{\nu'}=\Lambda_{\bar{\nu}}^{\bar{\nu}}\Lambda_{\nu''}^{\bar{\nu}'}\Lambda_{\nu''}^{\nu'}\Lambda_{\nu'}^{\nu}\frac{h_{\nu''}}{\sqrt{h_{\bar{\nu}}h_{\nu}}}\ . \tag{26b}$$

Notice that the two-body operator $V(k)=[a_l^{\dagger}\times a_l^{\dagger}]^k\cdot[\tilde{a}_l\times\tilde{a}_l]^k$ is a scalar of S_{n-2} and thus its matrix elements are diagonal in $\nu''\mu''$ and independent of the component index μ''. Using (24c) we have

$$\langle[\bar{\nu}]\bar{\alpha}L\|V(k)\|[\nu]\alpha L\rangle^{\bar{\nu}'\nu''\nu'}$$
$$=\sum_{\alpha''L''}(-)^{L''-L+k}\left[\frac{2L''+1}{2L+1}\right]^{1/2}\langle[\bar{\nu}]\bar{\alpha}L\|[a_l^{\dagger}\times a_l^{\dagger}]^k\|[\nu'']\alpha''L''\rangle^{\bar{\nu}'}\langle[\nu'']\alpha''L''\|[\tilde{a}_l\times\tilde{a}_l]^k\|[\nu]\alpha L\rangle^{\nu'}\ . \tag{26c}$$

Similar equation holds for the matrix element $\langle[\tilde{\bar{\nu}}]\bar{\beta}S\|V(q)\|[\tilde{\nu}]\beta S\rangle^{\tilde{\bar{\nu}}'\tilde{\nu}''\tilde{\nu}'}$.

E. The operators $[[a_l^{\dagger}\times a_l^{\dagger}]^k\times\tilde{a}_l]^{l'}$ and $[a_l^{\dagger}\times[\tilde{a}_l\times\tilde{a}_l]^k]^{l'}$

In the multishell calculation the matrix elements of the above two operators serve as two of the building blocks. Using (24c) we have

$$\langle[\bar{\nu}]\bar{\alpha}\bar{L}\|[[a_l^{\dagger}\times a_l^{\dagger}]^k\times\tilde{a}_l]^{l'}\|[\nu']\alpha'L'\rangle^{\bar{\nu}'\nu''}$$
$$=\sum_{\alpha''L''}(-)^{k+l-l'}U(L'l\bar{L}k;L''l')\langle[\bar{\nu}]\bar{\alpha}\bar{L}\|[a_l^{\dagger}\times a_l^{\dagger}]^k\|[\nu'']\alpha''L''\rangle^{\bar{\nu}'}\langle[\nu'']\alpha''L''\|\tilde{a}_l\|[\nu']\alpha'L'\rangle\ , \tag{27a}$$

$$\langle[\nu]\alpha L\|[a_l^{\dagger}\times[\tilde{a}_l\times\tilde{a}_l]^k]^{l'}\|[\nu^0]\alpha^0L^0\rangle^{\bar{\nu}\nu'}$$
$$=\sum_{\alpha'L'}(-)^{k+l-l'}U(L^0kLl;L'l')\langle[\nu]\alpha L\|a_l^{\dagger}\|[\nu']\alpha'L'\rangle\langle[\nu']\alpha'L'\|[\tilde{a}_l\times\tilde{a}_l]^k\|[\nu^0]\alpha^0L^0\rangle^{\bar{\nu}}\ . \tag{27b}$$

F. In the totally antisymmetric space

Since in the totally antisymmetric space the hybrid operators reduce to the fermion operators, the (l^ns^n) cases discussed above also cover the (γ^n) cases, where $\gamma=j$, or jt, which can be classified as the single-shell zero-spin case. The formulas (14.32)–(14.35) obtained through the second QF by Brussard and Glaudemans[9] are special cases of our (24c), (26c), and (27) [in conjunction with (16)–(18)]. By letting $l\to j$, $L\to J$, $[\nu]=[1^n],[\nu']=[1^{n-1}]$, and $[\nu'']=[1^{n-2}]$, Eqs. (24c), (26c), and (27) collapse to their results. In passing, we note that the factor $\sqrt{(n+1)n(n-1)}$ in their Eq. (14.33) is incorrect; it should be $(n-1)\sqrt{n}$ as shown in Eq. (18).

V. APPLICATION TO THE MULTISHELL, MULTISPIN CASE

It is sufficient to consider the two-shell, two-spin case, since the extension to the multishell, multispin case is straightforward. Let $\alpha_i,\beta_i,\ldots$ be the s.p. state labels for the shell i, e.g., $\alpha_i=l_im_i$, which span the defining representation of $U(M_i)$, $M_i=2l_i+1$. The definition of the hybrid operator $\alpha_i^\dagger$ is exactly the same as for the single-shell case, i.e., see Definition 2.

Definition 2. The operator $a_{\alpha_i}^\dagger$ (a_{α_i}) creates (annihilates) the last particle in the state α_i.

Similar to the single-shell case, the hybrid operators neither commute nor anticommute,

$$[a_{\alpha_i}^\dagger,a_{\alpha_j}^\dagger]_\pm\neq 0,\quad [a_{\alpha_i},a_{\alpha_j}]_\pm\neq 0 \quad \text{for any } i,j\ , \tag{28a}$$

and when acting on an antisymmetric state they satisfy

$$(n+1)a_{j_1m_1}\hat{a}_{j_2m_2}^\dagger+n\hat{a}_{j_2m_2}^\dagger a_{j_1m_1}=\delta_{j_1j_2}\delta_{m_1m_2}\ . \tag{28b}$$

A. The irreducible basis for the two-shell, two-spin case

The group chain $U(M)\supset O(3)$ for the single-shell case is extended to

$$\begin{array}{llllllll} U(M)\supset O(3) \rightarrow & U(M_1+M_2)\supset & (U(M_1)\supset O(3)) & \otimes & (U(M_2)\times O(3)) & \supset O(3) \\ [\nu] \quad \alpha LM \rightarrow & [\nu]\theta & [\nu_1] \quad \alpha_1L_1 & & [\nu_2] \quad \alpha_2L_2 & LM \end{array} \tag{29}$$

with $M_i=2l_i+1$, $i=1,2$. The multiplicity label α for the single shell goes over to

$$\alpha\rightarrow\theta[\nu_1]\alpha_1L_1,[\nu_2]\alpha_2L_2\ , \tag{30a}$$

where the quantum number θ is a multiplicity label,

$$\theta=1,2,\ldots,\{\nu_1\nu_2\nu\}\ , \tag{30b}$$

with the integer $\{\nu_1\nu_2\nu\}$ decided by the Littlewood rule. In the following the multiplicity labels α_1 and α_2 are suppressed for brevity.

The single-shell state is replaced by

$$|[\nu]\mu,\alpha LM\rangle\rightarrow\left|\begin{matrix}[\nu]\mu\theta LM\\ \nu_1L_1\nu_2L_2\end{matrix}\right\rangle\ . \tag{31a}$$

When we focus our attention to the unitary groups, it is convenient to introduce the $U(M_1+M_2)\supset U(M_1)\otimes U(M_2)$ basis

$$|\nu_1\nu_2,\nu\theta\rangle \tag{31b}$$

with all the SO(3) quantum numbers being totally ignored. The spaces spanned by the basis vectors (31a) and (31b) are referred to as $V^{M_1+M_2}$ and $\mathbb{V}^{M_1+M_2}$, respectively.

The basis (31a) has a definite symmetry for the group $U(M_1+M_2)$, and is referred to as the coupled basis. In contrast, the following basis is called a decoupled basis:

$$|\nu_1\mu_1L_1,\nu_2\mu_2L_2;LM\rangle\equiv|\nu_1\mu_1(1,2,\ldots,n_1)L_1,\nu_2\mu_2(n_1+1,\ldots,n)L_2;LM\rangle\ , \tag{31c}$$

where the shells 1 and 2 are decoupled in the $U(M_1+M_2)$ level [i.e., it is no longer an irreducible basis of the group $U(M_1+M_2)$], leaving only the angular momentum coupling intact.

Similarly, to go from the single-spin to two-spin case, we make the following substitutions:

$$\begin{array}{llllll} U(N)\supset U(2) \rightarrow & U(N_1N_2)\supset & (U(N_1)\supset U(2)) & \times & (U(N_2)\supset U(2)) \\ [\tilde{\nu}] \quad \beta SM_S \rightarrow & [\tilde{\nu}]\phi & [\nu_s] \quad \beta_sSM_S & & [\nu_t] \quad \beta_tTM_T \end{array}\ . \tag{32a}$$

For convenience in exposition, s and t will be referred to as the spin and isospin, respectively, although they could be any two unitary quantum numbers. The group $SU(N_1)[SU(N_2)]$ is the unitary group associated with the spin s (t), and N_1 (N_2) is the total numbers of s.p. states in the s (t) subspace.

The multiplicity label β for the single-spin case goes over to

$$\beta\rightarrow\phi[\nu_s]\beta_sS,[\nu_t]\beta_tT\ , \tag{32b}$$

where the quantum number ϕ is the multiplicity label whose range is decided by the Clebsch-Gordan series of the permutation group S_n,

$$\phi=1,2,\ldots,(\nu_s\nu_t\tilde{\nu})\ . \tag{32c}$$

In the following for brevity the multiplicity labels β_s and β_t are incorporated into S and T.

The many-particle state for the single-spin case is replaced by

$$|[\tilde{\nu}]\beta SM_S\rangle\rightarrow\left|\begin{matrix}[\tilde{\nu}]\phi\\ \nu_sSM_S\nu_tTM_T\end{matrix}\right\rangle\ , \tag{33a}$$

where for simplicity we ignored the Yamanouchi symbol. When we focus our attention to the unitary groups, it is convenient to introduce the $U(N_1N_2)\supset U(N_1)\times U(N_2)$ basis

$$|\nu_s \nu_t, \tilde{\nu}\phi\rangle \tag{33b}$$

with all the U(2) quantum numbers being totally ignored. The spaces spanned by the basis vectors (33a) and (33b) are referred to as $V^{N_1 N_2}$ and $\mathbb{V}^{N_1 N}$, respectively.

Notice that if the quantum numbers s and t are the spin and isospin, then ν_s and ν_t are redundant, since they are determined by S and T, respectively,

$$[\nu_s]=\left[\frac{n}{2}+S, \frac{n}{2}-S\right], \quad [\nu_t]=\left[\frac{n}{2}+T, \frac{n}{2}-T\right] . \tag{34}$$

B. The matrix elements

1. Single-particle creation operator

With the substitutions (31a) and (33a), the single-particle CFP in the total space, Eq. (22a), is extended to

$$\left[[1^n]; \begin{matrix}[\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2,\end{matrix} \begin{matrix}[\tilde{\nu}]\phi \\ \nu_S S \nu_t T\end{matrix} \left\| a^\dagger_{l_1 st} \right\| [1^{n-1}]; \begin{matrix}[\nu']\theta' L' \\ \nu'_1 L'_1 \nu_2 L_2,\end{matrix} \begin{matrix}[\tilde{\nu}']\phi' \\ \nu'_s S' \nu'_t T'\end{matrix}\right]$$
$$=(\nu|b^\dagger|\nu')\left\langle \begin{matrix}[\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2\end{matrix} \left\| a^\dagger_{l_1} \right\| \begin{matrix}[\nu']\theta' L' \\ \nu'_1 L'_1 \nu_2 L_2\end{matrix}\right\rangle \left\langle \begin{matrix}[\tilde{\nu}]\phi \\ \nu_s S \nu_t T\end{matrix} \left\| a^\dagger_{st} \right\| \begin{matrix}[\tilde{\nu}']\phi' \\ \nu'_s S' \nu'_t T'\end{matrix}\right\rangle . \tag{35}$$

The second factor in (35) is the ISF corresponding to the group chain (29), or the one-body CFP for the mixed configuration. According to (9-24) in Ref. 5, it can be factored as a product of the $U(M_1+M_2)\supset U(M_1)\otimes U(M_2)$ one-particle CFP, the CFP for shell 1 and an SO(3) recoupling coefficient,

$$\left\langle \begin{matrix}[\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2\end{matrix} \left\| a^\dagger_{l_1} \right\| \begin{matrix}[\nu']\theta' L' \\ \nu'_1 L'_1 \nu_2 L_2\end{matrix}\right\rangle$$
$$= C^{(\nu)\theta, \nu_1 \nu_2}_{(\nu')\theta' \nu'_1 \nu_2, [1][1][0]} (-)^{L-L'+L'_1-L_1}$$
$$\times U(L'_1 L_2 l_1 L; L' L_1) \langle \nu_1 L_1 \| a^\dagger_{l_1} \| \nu'_1 L'_1\rangle . \tag{36a}$$

Similar expression exists for the matrix elements of $a^\dagger_{l_2}$. The first factor in (36a) is the $U(M_1+M_2)\supset U(M_1)\otimes U(M_2)$ one-particle CFP, which is just the outer-product isoscalar factors (OISF) $C^{(\nu)\theta,(\nu')\theta'}_{\nu_1 \nu'_1, \nu_2 \nu_2}$ of the permutation group S_n.[5,17] It is convenient to introduce the following notation for the $U(M_1+M_2)\supset U(M_1)\otimes U(M_2)$ CFP or the OISF:

$$C^{(\nu)\theta, \nu_1 \nu_2}_{(\nu')\theta' \nu'_1 \nu_2, [1][1][0]} = C^{(\nu)\theta, (\nu')\theta'}_{\nu_1 \nu'_1, \nu_2 \nu_2}$$
$$= \langle \nu_1 \nu_2, \nu\theta | a^\dagger_1 | \nu'_1 \nu_2, \nu'\theta'\rangle$$
$$= \langle \nu'_1 \nu_2, \nu'\theta' | a_1 | \nu_1 \nu_2, \nu\theta\rangle , \tag{36b}$$

where the creation (annihilation) operator $a^\dagger_1$ (a_1) can be visualized as the operation of adding (removing) one box to (from) the Young diagram $[\nu'_1]$ ($[\nu_1]$). The OISF $\langle \nu_1 \nu_2, \nu\theta | a^\dagger_1 | \nu'_1 \nu_2, \nu'\theta'\rangle$ gives the probability amplitude for the final state to be $|\nu_1 \nu_2, \nu\theta\rangle$ after adding a particle in the shell 1 to the state $|\nu'_1 \nu_2, \nu'\theta'\rangle$.

In order to give a physical interpretation of the factorization (36a) and simplify the derivation to be given later for the matrix elements of one- or two-body operators, we introduce the hybrid creation (annihilation) operator $\mathbb{a}^\dagger_{\alpha_i}$ ($\mathbb{a}_{\alpha_i}$) for the decoupled basis (31c). Notice that the shadowed symbol is used here to distinguish it from the operator defined by Definition 2.

Definition 3. The operator $\mathbb{a}^\dagger_{\alpha_i}$ ($\mathbb{a}_{\alpha_i}$) creates (annihilates) the last particle in the shell i with state label α_i in the decoupled basis. For example, we have

$$\mathbb{a}^\dagger_{\alpha_1}|\Psi(1,\ldots,n_1-1)\Phi(n_1+1,\ldots,n)\rangle$$
$$=|\Psi(1,\ldots,n_1-1)\psi_{\alpha_1}(n_1)\Phi(n_1+1,\ldots,n)\rangle ,$$
$$\mathbb{a}^\dagger_{\alpha_2}|\Psi(1,\ldots,n_1)\Phi(n_1+1,\ldots,n)\rangle$$
$$=|\Psi(1,\ldots,n_1)\Phi(n_1+1,\ldots,n)\phi_{\alpha_2}(n+1)\rangle ,$$
$$\mathbb{a}_{\alpha_1}|\Psi(1,\ldots,n_1-1)\psi_{\beta_1}(n_1)\Phi(n_1+1,\ldots,n)\rangle$$
$$=\delta_{\alpha_1\beta_1}|\Psi(1,\ldots,n_1-1)\Phi(n_1+1,\ldots,n)\rangle , \tag{37a}$$
$$\mathbb{a}_{\alpha_2}|\Psi(1,\ldots,n_1)\Phi(n_1+1,\ldots,n-1)\phi_{\beta_2}(n)\rangle$$
$$=\delta_{\alpha_2\beta_2}|\Psi(1,\ldots,n_1)\Phi(n_1+1,\ldots,n-1)\rangle ,$$

where Ψ and Φ are the wave functions for shells 1 and 2, respectively. Notice the subtle difference between Definitions 2 and 3. Clearly, the shadowed operators belonging to different shells commute with one another.

$$[\mathbb{a}_{\alpha_i}, \mathbb{a}^\dagger_{\alpha_j}]=[\mathbb{a}^\dagger_{\alpha_i}, \mathbb{a}^\dagger_{\alpha_j}]=[\mathbb{a}_{\alpha_i}, \mathbb{a}_{\alpha_j}]=0 \quad \text{for } i\neq j . \tag{37b}$$

Notice the essential difference between (28a) and (37b).

With the shadowed operator, (36a) can be rewritten as

$$\left\langle \begin{matrix}[\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2\end{matrix} \left\| a^\dagger_{l_1} \right\| \begin{matrix}[\nu']\theta' L' \\ \nu'_1 L'_1 \nu_2 L_2\end{matrix}\right\rangle$$
$$= \langle \nu_1 \nu_2, \nu\theta | a^\dagger_1 | \nu'_1 \nu_2, \nu'\theta'\rangle$$
$$\times \langle \nu_1 L_1 \nu_2 L_2; L \| \mathbb{a}^\dagger_{l_1} \| \nu'_1 L'_1 \nu_2 L_2; L'\rangle , \tag{38a}$$

$$\langle \nu_1 L_1 \nu_2 L_2; L \| \mathbb{a}^\dagger_{l_1} \| \nu'_1 L'_1 \nu_2 L_2; L'\rangle$$
$$=(-)^{L-L'+L'_1-L_1} U(L'_1 L_2 l_1 L; L' L_1)$$
$$\times \langle \nu_1 L_1 \| a^\dagger_{l_1} \| \nu'_1 L'_1\rangle . \tag{38b}$$

Equation (38a) can be interpreted in the following way: The OISF *undo the coupling* $[\nu_1]\otimes[\nu_2]\to[\nu]$ *between shell 1 and shell 2,* leaving only the angular-momentum coupling, while the matrix elements of the shadowed operator $\mathbb{a}_{l_1}^\dagger$ in the decoupled basis can be calculated by simply using the Racah algebra.

Equation (37b) enables us to reorder the creation and annihilation operators belonging to different shells (in conjunction of course with the corresponding change in angular momentum coupling). This property is crucial for the multishell calculation.

Notice that for a single shell, the shadowed and plain-faced operators are identical. To simplify the notation, henceforth we will not distinguish these two symbols. Depending on which basis (coupled or decoupled) they are acting, we immediately know which is which.

The last factor in (35) is the ISF corresponding to the group chain (32a). According to (7-153) in Ref. 5 and in parallel with (38a), we have

$$\left\langle \begin{matrix}[\tilde{\nu}]\phi \\ \nu_s S \nu_t T\end{matrix} \middle\| a_{st}^\dagger \middle\| \begin{matrix}[\tilde{\nu}']\phi' \\ \nu_s' S' \nu_t' T'\end{matrix} \right\rangle = \langle \nu_s\nu_t, \tilde{\nu}\phi | b^\dagger | \nu_s'\nu_t', \tilde{\nu}'\phi' \rangle \langle \nu_s S \| a_s^\dagger \| \nu_s' S' \rangle \times \langle \nu_t T \| a_t^\dagger \| \nu_t' T' \rangle , \tag{39a}$$

where the first factor is the $U(N_1N_2)\supset U(N_1)\times U(N_2)$ one-particle CFP, which is just the inner-product isoscalar factor (IISF) $C^{(\nu)\phi,(\nu')\phi'}_{\nu_s\nu_s',\nu_t\nu_t'}$ of the permutation group[5,15]

$$\langle \nu_s\nu_t, \nu\phi | b^\dagger | \nu_s'\nu_t', \nu'\phi' \rangle = \langle \nu_s'\nu_t', \nu'\phi' | b | \nu_s\nu_t, \nu\phi \rangle = C^{(\nu)\phi,(\nu')\phi'}_{\nu_s\nu_s',\nu_t\nu_t'} . \tag{39b}$$

The IISF undo the coupling $[\nu_s]\times[\nu_t]\to[\tilde{\nu}]$ between the spin spaces V^{N_1} and the isospin space V^{N_2}, and is the probability amplitude for the final state to be $|\nu_s\nu_t, \tilde{\nu}\phi\rangle$ after adding one particle to the state $|\nu_s'\nu_t', \tilde{\nu}'\phi'\rangle$. The CFP in (22b) is a special case of (39b). If s and t are the usual spin and isospin, then the quantity in (39b) is the spin-isospin one-particle CFP. An efficient code is available for the OISF and IISF.[18]

The factorization (35) for a single creation operator can be generalized to any product of the creation and annihilation operators. Below are the matrix elements of the one- and two-body operators.

2. One-body operator

Equation (24a) is extended to

$$\left\{ [1^n];\ \begin{matrix}[\bar{\nu}]\bar{\theta}\bar{L} \\ \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2\end{matrix} ,\ \begin{matrix}[\bar{\tilde{\nu}}']\bar{\phi} \\ \bar{\nu}_s\bar{S}\bar{\nu}_t\bar{T}\end{matrix} \middle\| [a_{l_i st}^\dagger \times \tilde{a}_{l_j st}]^{kqr} \middle\| [1^n];\ \begin{matrix}[\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2\end{matrix} ,\ \begin{matrix}[\tilde{\nu}]\phi \\ \nu_s S \nu_t T\end{matrix} \right\}$$

$$= \sum_{\nu'} (\bar{\nu}|b^\dagger b|\nu)_{\nu'} \left\langle \begin{matrix}[\bar{\nu}]\bar{\theta}\bar{L} \\ \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2\end{matrix} \middle\| [a_{l_i}^\dagger \times \tilde{a}_{l_j}]^k \middle\| \begin{matrix}[\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2\end{matrix} \right\rangle^{\nu'} \left\langle \begin{matrix}[\bar{\tilde{\nu}}]\bar{\phi} \\ \bar{\nu}_s\bar{S}\bar{\nu}_t\bar{T}\end{matrix} \middle\| [a_{st}^\dagger \times \tilde{a}_{st}]^{qr} \middle\| \begin{matrix}[\tilde{\nu}]\phi \\ \nu_s S \nu_t T\end{matrix} \right\rangle^{\tilde{\nu}'} . \tag{40}$$

The second factor in (40) is the one-body matrix element in the space $V^{M_1+M_2}$, which can be factored as

$$\left\langle \begin{matrix}[\bar{\nu}]\bar{\theta}\bar{L} \\ \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2\end{matrix} \middle\| [a_{l_i}^\dagger \times \tilde{a}_{l_j}]^k \middle\| \begin{matrix}[\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2\end{matrix} \right\rangle^{\nu'} = \sum_{(\nu_1\nu_2)_{\rm int}} \langle \bar{\nu}_1\bar{\nu}_2, \bar{\nu}\bar{\theta} | a_i^\dagger a_j | \nu_1\nu_2, \nu\theta \rangle^{\nu'}_{(\nu_1\nu_2)_{\rm int}} \langle \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2;\bar{L} \| [a_{l_i}^\dagger \times \tilde{a}_{l_j}]^k \| \nu_1 L_1 \nu_2 L_2; L \rangle^{(\nu_1\nu_2)_{\rm int}} , \tag{41}$$

where $(\nu_1\nu_2)_{\rm int}$ is the shorthand notation for the irrep labels of the intermediate states, which specify the path for the further factorization of the two matrix elements in (41). The matrix elements $\langle \bar{\nu}_1\bar{\nu}_2, \bar{\nu}\bar{\theta} | a_i^\dagger a_j | \nu_1\nu_2, \nu\theta \rangle^{\nu'}_{(\nu_1\nu_2)_{\rm int}}$ undo the coupling between shell 1 and shell 2, and is called the one-body matrix element in the space $\mathbb{V}^{M_1+M_2}$. By inserting a complete set of intermediate states and noting that the quantum numbers ν' and $(\nu_1\nu_2)_{\rm int}$ have already specified the irrep labels of the intermediate states, we have

$$\langle \bar{\nu}_1\nu_2, \bar{\nu}\bar{\theta} | a_1^\dagger a_1 | \nu_1\nu_2, \nu\theta \rangle^{\nu'}_{\nu_1'} = \sum_{\theta'} \langle \bar{\nu}_1\nu_2, \bar{\nu}\bar{\theta} | a_1^\dagger | \nu_1'\nu_2, \nu'\theta' \rangle \langle \nu_1'\nu_2, \nu'\theta' | a_1 | \nu_1\nu_2, \nu\theta \rangle , \tag{42a}$$

$$\langle \nu_1^0\nu_2', \bar{\nu}\bar{\theta} | a_1^\dagger a_2 | \nu_1\nu_2, \nu\theta \rangle^{\nu'} = \sum_{\theta'} \langle \nu_1^0\nu_2', \bar{\nu}\bar{\theta} | a_1^\dagger | \nu_1\nu_2', \nu'\theta' \rangle \langle \nu_1\nu_2', \nu'\theta' | a_2 | \nu_1\nu_2, \nu\theta \rangle , \tag{42b}$$

$$\langle \nu_1'\nu_2^0, \bar{\nu}\bar{\theta} | a_2^\dagger a_1 | \nu_1\nu_2, \nu\theta \rangle^{\nu'} = \sum_{\theta'} \langle \nu_1'\nu_2^0, \bar{\nu}\bar{\theta} | a_2^\dagger | \nu_1'\nu_2, \nu'\theta' \rangle \langle \nu_1'\nu_2, \nu'\theta' | a_1 | \nu_1\nu_2, \nu\theta \rangle . \tag{42c}$$

The orbital matrix elements $\langle \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2;\bar{L} \| [a_{l_i}^\dagger \times \tilde{a}_{l_j}]^k \| \nu_1 L_1 \nu_2 L_2; L \rangle^{(\nu_1\nu_2)_{\rm int}}$ in the decoupled basis can be calculated by simply using the Racah algebra and will not be given here.

The last factor in (40) is the one-body matrix element in the space $V^{N_1N_2}$, which, in analogy with Eq. (41), is factored as

$$\left\langle \begin{matrix} [\tilde{\bar{\nu}}]\phi \\ \bar{\nu}_s\bar{S}\bar{\nu}_t\bar{T} \end{matrix} \middle| [a_{st}^\dagger \times a_{st}]^{qr} \middle| \begin{matrix} [\tilde{\nu}]\phi \\ \nu_s S \nu_t T \end{matrix} \right\rangle^{\bar{\nu}'} = \sum_{\nu_s'\nu_t'} \langle \bar{\nu}_s\bar{\nu}_t, \tilde{\bar{\nu}}\bar{\phi} | b^\dagger b | \nu_s\nu_t, \tilde{\nu}\phi \rangle_{\nu_s'\nu_t'}^{\bar{\nu}'} \langle \bar{\nu}_s\bar{S}\bar{\nu}_t\bar{T} \| [a_{st}^\dagger \times \tilde{a}_{st}]^{qr} \| \nu_s S \nu_t T \rangle^{\nu_s'\nu_t'} . \tag{43}$$

The factor $\langle \bar{\nu}_s\bar{\nu}_t, \tilde{\bar{\nu}}\bar{\phi} | b^\dagger b | \nu_s\nu_t, \tilde{\nu}\phi \rangle_{\nu_s'\nu_t'}^{\bar{\nu}'}$ is the one-body matrix element in the space $\mathbb{V}^{N_1N_2}$, which decouples the spin space V^{N_1} from the isospin space V^{N_2}. In analogy with Eq. (42) we have the following factorization:

$$\langle \bar{\nu}_s\bar{\nu}_t, \tilde{\bar{\nu}}\bar{\phi} | b^\dagger b | \nu_s\nu_t, \tilde{\nu}\phi \rangle_{\nu_s'\nu_t'}^{\bar{\nu}'} = \sum_{\phi'} \langle \bar{\nu}_s\bar{\nu}_t, \tilde{\bar{\nu}}\bar{\phi} | b^\dagger | \nu_s'\nu_t', \tilde{\nu}'\phi' \rangle \langle \nu_s'\nu_t', \tilde{\nu}'\phi' | b | \nu_s\nu_t, \tilde{\nu}\phi \rangle . \tag{44}$$

The second factor in (43) is simply the product of the one-body matrix elements in the spaces V^{N_1} and V^{N_2},

$$\langle \bar{\nu}_s\bar{S}\bar{\nu}_t\bar{T} \| [a_{st}^\dagger \times \tilde{a}_{st}]^{qr} \| \nu_s S \nu_t T \rangle^{\nu_s'\nu_t'} = \langle \bar{\nu}_s\bar{S} \| [a_s^\dagger \times \tilde{a}_s]^q \| \nu_s S \rangle^{\nu_s'} \langle \bar{\nu}_t\bar{T} \| [a_t^\dagger \times \tilde{a}_t]^r \| \nu_t T \rangle^{\nu_t'} . \tag{43'}$$

Notice that when $\tilde{\nu}$ (and thus $\tilde{\nu}'$) is totally antisymmetric, (43) is reduced to (24a) by letting $\nu_s' = \tilde{\nu}_t' \to \nu'$, $(st) \to (ls)$, and $(qr) \to (kq)$.

3. *Two-body operator:* $V(kqr) = [a_{l_i st}^\dagger \times a_{l_j st}^\dagger]^{kqr} \cdot [\tilde{a}_{l_{j'} st} \times \tilde{a}_{l_{i'} st}]^{kqr}$

Equation (26a) is generalized to

$$\left[[1^n]; \begin{matrix} [\bar{\nu}]\bar{\theta}L \\ \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2 \end{matrix} , \begin{matrix} [\tilde{\bar{\nu}}]\bar{\phi} \\ \bar{\nu}_s\bar{S}\bar{\nu}_t\bar{T} \end{matrix} \middle\| V(kqr) \middle\| [1^n]; \begin{matrix} [\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2 \end{matrix} , \begin{matrix} [\tilde{\nu}]\phi \\ \nu_s S \nu_t T \end{matrix} \right]$$

$$= \sum_{\bar{\nu}'\nu''\nu'} (\bar{\nu} | b^\dagger b^\dagger b b | \nu)_{\bar{\nu}'\nu''\nu'} \left\langle \begin{matrix} [\bar{\nu}]\bar{\theta}L \\ \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2 \end{matrix} \middle\| V(k) \middle\| \begin{matrix} [\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2 \end{matrix} \right\rangle^{\bar{\nu}'\nu''\nu'} \left\langle \begin{matrix} [\tilde{\bar{\nu}}]\phi \\ \bar{\nu}_s\bar{S}\bar{\nu}_t\bar{T} \end{matrix} \middle\| V(qr) \middle\| \begin{matrix} [\tilde{\nu}]\phi \\ \nu_s S \nu_t T \end{matrix} \right\rangle^{\tilde{\bar{\nu}}'\tilde{\nu}''\tilde{\nu}'} , \tag{45}$$

where

$$V(k) = [a_{l_i}^\dagger \times a_{l_j}^\dagger]^k \cdot [\tilde{a}_{l_{j'}} \times \tilde{a}_{l_{i'}}]^k, \quad V(qr) = [a_{st}^\dagger \times a_{st}^\dagger]^{qr} \cdot [\tilde{a}_{st} \times \tilde{a}_{st}]^{qr} . \tag{46}$$

The second factor in (45) is the two-body matrix element in the space $V^{M_1+M_2}$, which is again factored

$$\left\langle \begin{matrix} [\bar{\nu}]\bar{\theta}L \\ \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2 \end{matrix} \middle\| V(k) \middle\| \begin{matrix} [\nu]\theta L \\ \nu_1 L_1 \nu_2 L_2 \end{matrix} \right\rangle^{\bar{\nu}'\nu''\nu'}$$

$$= \sum_{(\nu_1\nu_2)_{\text{int}}} \langle \bar{\nu}_1\bar{\nu}_2, \bar{\nu}\bar{\theta} | a_i^\dagger a_j^\dagger a_{j'} a_{i'} | \nu_1\nu_2, \nu\theta \rangle_{(\nu_1\nu_2)_{\text{int}}}^{\bar{\nu}'\nu''\nu'} \langle \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2; L \| V(k) \| \nu_1 L_1 \nu_2 L_2; L \rangle^{(\nu_1\nu_2)_{\text{int}}} . \tag{47}$$

The intermediate quantum numbers $(\nu_1\nu_2)_{\text{int}}$ are determined by the combinations of the indices i, j, j', and i'. The first factor in (47) is the two-body matrix elements in the space $\mathbb{V}^{M_1+M_2}$, which can be expressed as a sum of products of four OISF. Some typical cases for them are listed below:

$$\langle \bar{\nu}_1\nu_2, \bar{\nu}\bar{\theta} | a_1^\dagger a_1^\dagger a_1 a_1 | \nu_1\nu_2, \nu\theta \rangle_{\bar{\nu}_1'\nu_1''\nu_1'}^{\bar{\nu}'\nu''\nu'} = \sum_{\bar{\theta}'\theta''\theta'} \langle \bar{\nu}_1\nu_2, \bar{\nu}\bar{\theta} | a_1^\dagger | \bar{\nu}_1'\nu_2, \bar{\nu}'\bar{\theta}' \rangle \langle \bar{\nu}_1'\nu_2, \bar{\nu}'\bar{\theta}' | a_1^\dagger | \nu_1''\nu_2, \nu''\theta'' \rangle$$
$$\times \langle \nu_1''\nu_2, \nu''\theta'' | a_1 | \nu_1'\nu_2, \nu'\theta' \rangle \langle \nu_1'\nu_2, \nu'\theta' | a_1 | \nu_1\nu_2, \nu\theta \rangle , \tag{48a}$$

$$\langle \nu_1^{00}\nu_2'', \bar{\nu}\bar{\theta} | a_1^\dagger a_1^\dagger a_2 a_2 | \nu_1\nu_2, \nu\theta \rangle_{\nu_1^0\nu_2'}^{\bar{\nu}'\nu''\nu'} = \sum_{\bar{\theta}'\theta''\theta'} \langle \nu_1^{00}\nu_2'', \bar{\nu}\bar{\theta} | a_1^\dagger | \nu_1^0\nu_2'', \bar{\nu}'\bar{\theta}' \rangle \langle \nu_1^0\nu_2'', \bar{\nu}'\bar{\theta}' | a_1^\dagger | \nu_1\nu_2'', \nu''\theta'' \rangle$$
$$\times \langle \nu_1\nu_2'', \nu''\theta'' | a_2 | \nu_1\nu_2', \nu'\theta' \rangle \langle \nu_1\nu_2', \nu'\theta' | a_2 | \nu_1\nu_2, \nu\theta \rangle , \tag{48b}$$

$$\langle \bar{\nu}_1\bar{\nu}_2, \bar{\nu}\bar{\theta} | a_1^\dagger a_2^\dagger a_2 a_1 | \nu_1\nu_2, \nu\theta \rangle_{\nu_1'\nu_2'}^{\bar{\nu}'\nu''\nu'} = \sum_{\bar{\theta}'\theta''\theta'} \langle \bar{\nu}_1\bar{\nu}_2, \bar{\nu}\bar{\theta} | a_1^\dagger | \nu_1'\bar{\nu}_2, \bar{\nu}'\bar{\theta}' \rangle \langle \nu_1'\bar{\nu}_2, \bar{\nu}'\bar{\theta}' | a_2^\dagger | \nu_1'\nu_2', \nu''\theta'' \rangle$$
$$\times \langle \nu_1'\nu_2', \nu''\theta'' | a_2 | \nu_1'\nu_2, \nu'\theta' \rangle \langle \nu_1'\nu_2, \nu'\theta' | a_1 | \nu_1\nu_2, \nu\theta \rangle , \tag{48c}$$

$$\langle \nu_1^0\nu_2', \bar{\nu}\bar{\theta} | a_1^\dagger a_1^\dagger a_1 a_2 | \nu_1\nu_2, \nu\theta \rangle_{\bar{\nu}_1\nu_1'}^{\bar{\nu}'\nu''\nu'} = \sum_{\bar{\theta}'\theta''\theta'} \langle \nu_1^0\nu_2', \bar{\nu}\bar{\theta} | a_1^\dagger | \bar{\nu}_1\nu_2', \bar{\nu}'\bar{\theta}' \rangle \langle \bar{\nu}_1\nu_2', \bar{\nu}'\bar{\theta}' | a_1^\dagger | \nu_1'\nu_2', \nu''\theta'' \rangle$$
$$\times \langle \nu_1'\nu_2', \nu''\theta'' | a_1 | \nu_1\nu_2', \nu'\theta' \rangle \langle \nu_1\nu_2', \nu'\theta' | a_2 | \nu_1\nu_2, \nu\theta \rangle , \tag{48d}$$

$$\langle \nu_1^0\bar{\nu}_2',\bar{\nu}\bar{\theta}|a_1^\dagger a_2^\dagger a_2 a_2|\nu_1\nu_2,\nu\theta\rangle_{\nu_2'\nu_2''}^{\bar{\nu}'\nu''\nu'}=\sum_{\bar{\theta}'\theta''\theta'}\langle \nu_1^0\bar{\nu}_2',\bar{\nu}\bar{\theta}|a_1^\dagger|\nu_1\bar{\nu}_2',\bar{\nu}'\bar{\theta}'\rangle\langle \nu_1\bar{\nu}_2',\bar{\nu}'\bar{\theta}'|a_2^\dagger|\nu_1\nu_2'',\nu''\theta''\rangle \times\langle \nu_1\nu_2'',\nu''\theta''|a_2|\nu_1\nu_2',\nu'\theta'\rangle\langle \nu_1\nu_2',\nu'\theta'|a_2|\nu_1\nu_2,\nu\theta\rangle\ . \tag{48e}$$

The corresponding matrix elements $\langle \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2;L\|V(k)\|\nu_1L_1\nu_2L_2;L\rangle^{(\nu_1\nu_2)_{\rm int}}$ in the orbital space can be calculated by the Racah algebra as follows.

(a) $V(k)=V_{11,11}^k\equiv[a_{l_1}^\dagger\times a_{l_1}^\dagger]^k\cdot[\tilde{a}_{l_1}\times\tilde{a}_{l_1}]^k$

$$\langle \bar{\nu}_1\bar{L}_1\nu_2L_2;L\|V_{11,11}^k\|\nu_1L_1\nu_2L_2;L\rangle^{\bar{\nu}_1'\nu_1''\nu_1'}=\langle \bar{\nu}_1\bar{L}_1\|V_{11,11}^k\|\nu_1L_1\rangle^{\bar{\nu}_1'\nu_1''\nu_1'}\delta_{\bar{L}_1L_1}\ . \tag{49a}$$

(b) $V(k)=V_{11,22}^k\equiv[a_{l_1}^\dagger\times a_{l_1}^\dagger]^k\cdot[\tilde{a}_{l_2}\times\tilde{a}_{l_2}]^k$

$$\langle \bar{\nu}_1\bar{L}_1\nu_2''L_2'';L\|V_{11,22}^k\|\nu_1L_1\nu_2L_2;L\rangle^{\nu_1^0\nu_2'}=(-)^{\bar{L}_1+L_2-L-k}\hat{\bar{L}}_1\hat{L}_2''W(\bar{L}_1L_2''L_1L_2;Lk) \times\langle \bar{\nu}_1\bar{L}_1\|[a_{l_1}^\dagger\times a_{l_1}^\dagger]^k\|\nu_1L_1\rangle^{\nu_1^0}\langle \nu_2''L_2''\|[\tilde{a}_{l_2}\times\tilde{a}_{l_2}]^k\|\nu_2L_2\rangle^{\nu_2'}\ , \tag{49b}$$

where $\hat{L}=\sqrt{2L+1}$.

(c) $V(k)=V_{12,21}^k\equiv[a_{l_1}^\dagger\times a_{l_2}^\dagger]^k\cdot[\tilde{a}_{l_2}\times\tilde{a}_{l_1}]^k$.

Using the fact that in the decoupled basis, the generalized operators belonging to different shells commute [see Eq. (37b)], we have the identity

$$[a_{l_1}^\dagger\times a_{l_2}^\dagger]^k\cdot[\tilde{a}_{l_2}\times\tilde{a}_{l_1}]^k=(-)^{k-l_1-l_2}[a_{l_1}^\dagger\times a_{l_2}^\dagger]^k\cdot[\tilde{a}_{l_1}\times\tilde{a}_{l_2}]^k =\sum_\lambda(-)^\lambda\frac{\hat{k}}{\hat{\lambda}}U(l_1l_2l_1l_2;k\lambda)[a_{l_1}^\dagger\times\tilde{a}_{l_1}]^\lambda\cdot[a_{l_2}^\dagger\times\tilde{a}_{l_2}]^\lambda\ . \tag{50}$$

Using the above equation, the matrix element of the operator $V_{12,21}^k$ can be expressed in terms of the one-body matrix elements for shell 1 and shell 2,

$$\langle \bar{\nu}_1\bar{L}_1\bar{\nu}_2\bar{L}_2;L\|V_{12,21}^k\|\nu_1L_1\nu_2L_2;L\rangle^{\nu_1'\nu_2'}=\sum_\lambda(-)^{\bar{L}_1+L_2-L}\frac{\hat{k}}{\hat{\lambda}}U(l_1l_2l_1l_2;k\lambda)\hat{\bar{L}}_1\hat{\bar{L}}_2W(\bar{L}_1\bar{L}_2L_1L_2;L\lambda) \times\langle \bar{\nu}_1\bar{L}_1\|[a_{l_1}^\dagger\times\tilde{a}_{l_1}]^\lambda\|\nu_1L_1\rangle^{\nu_1'}\langle \bar{\nu}_2\bar{L}_2\|[a_{l_2}^\dagger\times\tilde{a}_{l_2}]^\lambda\|\nu_2L_2\rangle^{\nu_2'}\ . \tag{49c}$$

(d) $V(k)=V_{11,12}^k\equiv[[a_{l_1}^\dagger\times a_{l_1}^\dagger]^k\times\tilde{a}_{l_1}]^{l_2}\cdot\tilde{a}_{l_2}=\frac{\hat{l}_2}{\hat{k}}[a_{l_1}^\dagger\times a_{l_1}^\dagger]^k\cdot[\tilde{a}_{l_1}\times\tilde{a}_{l_2}]^k$

$$\langle \nu_1^0L_1^0\nu_2'L_2';L\|V_{11,12}^k\|\nu_1L_1\nu_2L_2;L\rangle^{\bar{\nu}_1\nu_1'} =(-)^{L_1^0+L_2-L-l_2}\hat{L}_1^0\hat{L}_2'W(L_1^0L_2'L_1L_2;Ll_2)\langle \nu_1^0L_1^0\|[[a_{l_1}^\dagger\times a_{l_1}^\dagger]^k\times\tilde{a}_{l_1}]^{l_2}\|\nu_1L_1\rangle^{\bar{\nu}_1\nu_1'}\langle \nu_2'L_2'\|\tilde{a}_{l_2}\|\nu_2L_2\rangle\ . \tag{49d}$$

(e) $V(k)=V_{12,22}^k\equiv a_{l_1}^\dagger\cdot[a_{l_2}^\dagger\times[\tilde{a}_{l_2}\times\tilde{a}_{l_2}]^k]^{l_1}=\frac{\hat{l}_1}{\hat{k}}[a_{l_1}^\dagger\times a_{l_2}^\dagger]^k\cdot[\tilde{a}_{l_2}\times\tilde{a}_{l_2}]^k$

$$\langle \nu_1^0L_1^0\bar{\nu}_2'\bar{L}_2';L\|V_{12,22}^k\|\nu_1L_1\nu_2L_2;L\rangle^{\nu_2'\nu_2''} =(-)^{L_1^0+L_2-L-l_1}\hat{L}_1^0\hat{\bar{L}}_2'W(L_1^0\bar{L}_2'L_1L_2;Ll_1)\langle \nu_1^0L_1^0\|a_{l_1}^\dagger\|\nu_1L_1\rangle\langle \bar{\nu}_2'\bar{L}_2'\|[a_{l_2}^\dagger\times[\tilde{a}_{l_2}\times\tilde{a}_{l_2}]^k]^{l_1}\|\nu_2L_2\rangle^{\nu_2'\nu_2''}\ . \tag{49e}$$

In analogy with (47), the two-body matrix elements in the spin-isospin space $V^{N_1N_2}$ is factored

$$\left\langle {[\bar{\nu}]\bar{\phi} \atop \bar{\nu}_S S\bar{\nu}_t T}\right\|V(qr)\left\|{[\nu]\phi \atop \nu_s S\nu_t T}\right\rangle^{\bar{\nu}'\nu''\nu'}=\sum_{\bar{\nu}_s'\nu_s''\nu_s'}\sum_{\bar{\nu}_t'\nu_t''\nu_t'}\langle \bar{\nu}_s\bar{\nu}_t,\bar{\nu}\bar{\phi}|b^\dagger b^\dagger bb|\nu_s\nu_t,\bar{\nu}\phi\rangle_{\bar{\nu}_s'\nu_s''\nu_s',\bar{\nu}_t'\nu_t''\nu_t'}^{\bar{\nu}'\nu''\bar{\nu}'} \times\langle \bar{\nu}_sS\|V(q)\|\nu_sS\rangle^{\bar{\nu}_s'\nu_s''\nu_s'}\langle \bar{\nu}_tT\|V(r)\|\nu_tT\rangle^{\bar{\nu}_t'\nu_t''\nu_t'}\ . \tag{50a}$$

Similar to Eq. (48), the two-body matrix elements in $\mathbb{V}^{N_1N_2}$ can be expressed as a sum of products of four IISF,

$$\langle \bar{\nu}_s\bar{\nu}_t,\bar{\nu}\bar{\phi}|b^\dagger b^\dagger bb|\nu_s\nu_t,\bar{\nu}\phi\rangle_{\bar{\nu}_s'\nu_s''\nu_s',\bar{\nu}_t'\nu_t''\nu_t'}^{\bar{\nu}'\nu''\bar{\nu}'} =\sum_{\bar{\phi}'\phi''\phi'}\langle \bar{\nu}_s\bar{\nu}_t,\bar{\nu}\bar{\phi}|b^\dagger|\bar{\nu}_s'\bar{\nu}_t',\bar{\nu}'\bar{\phi}'\rangle\langle \bar{\nu}_s'\bar{\nu}_t',\bar{\nu}'\bar{\phi}'|b^\dagger|\nu_s''\nu_t'',\bar{\nu}''\phi''\rangle\langle \nu_s''\nu_t'',\bar{\nu}''\phi''|b|\nu_s'\nu_t',\bar{\nu}'\phi'\rangle\langle \nu_s'\nu_t',\bar{\nu}'\phi'|b|\nu_s\nu_t,\bar{\nu}\phi\rangle\ . \tag{50b}$$

Notice that when $\bar{\nu}$ (and thus $\tilde{\bar{\nu}}', \bar{\nu}'', \bar{\nu}'$) is totally antisymmetric, (50a) is reduced to (26a) by letting $\bar{\nu}_s' = \tilde{\bar{\nu}}_t' \to \bar{\nu}'$, $\nu_s'' = \tilde{\nu}_t'' \to \nu''$, $\nu_s' = \tilde{\nu}_t' \to \nu'$, $(st) \to (ls)$, and $(qr) \to (kq)$.

C. In the totally antisymmetric space

To conform with the conventional notation of using jm as the single-particle state label in a totally antisymmetric space, in this subsection we change the notation $\alpha_i \to j_i m_i$, $l_i \to j_i$, $L_i \to J_i$.

Brussaard and Glaudemans[9] obtained the formulas for the two-shell matrix elements of a two-body operator using both the first QF (a diagrammatical method, i.e., antisymmetrization by brutal force) and second QF by lengthy derivation. To apply our general formula to the totally antisymmetric case, we need the following special OISF. From (4-163) and (7-254b) in Ref. 5 we have

$$([1^{n_1}][1^{n_2}],[1^n]|a_1^\dagger|[1^{n_1-1}][1^{n_2}],[1^{n-1}]) = (-)^{n_2}\sqrt{n_1/n} , \quad (51a)$$

$$([1^{n_1}][1^{n_2}],[1^n]|a_2^\dagger|[1^{n_1}][1^{n_2-1}],[1^{n-1}]) = \sqrt{n_2/n} , \quad (51b)$$

where $n = n_1 + n_2$.

It can be shown that Brussaard and Glaudemans's formulas (5.33) and (5.40) of Ref. 9 are just *trivial* cases of our (49a) and (49c), while their (5.78) and (5.74) are *trivial* cases of our (49b), (49d), and (49e); namely, the case they treated corresponds to our two-shell, zero-spin case. Their Eq. (15.15) obtained by second QF is a special case of (49a) and (49c) here. Their Eq. (14.9) is a direct result of Eqs. (47) and (51). To show this let us derive the phase factor $(-)^{(n_1+n_1')n_2}$ in (14.9) of Ref. 9, since other factors are easily obtained.

Suppose that in the n-body operator there are $\mathfrak{m}_1$ creation and/or annihilation operators $a_1^\dagger \cdots a_1$ and $\mathfrak{m}_2$ operators $a_2^\dagger \cdots a_2$. According to (51) and their Hermitian conjugate we know that only the matrix element of $a_1^\dagger$ or a_1 contributes a sign $(-)^{n_2}$. Therefore

$$(n\text{-body matrix elements in } \mathbb{V}^{M_1+M_2}) = ([1^{n_1}][1^{n_2}],[1^n]|a_1^\dagger \cdots a_1 a_2^\dagger \cdots a_2|[1^{n_1'}][1^{n_2'}],[1^n]) = (-)^{\mathfrak{m}_1 n_2} C = (-)^{(n_1+n_1')n_2} C ,$$

where we used the fact that if $\mathfrak{m}_1$ is even (or odd), so is $n_1 + n_1'$ and C is a coefficient.

As a further check in the following we calculate the matrix element of the two-body operator

$$V_{11,12}^k = [a_{j_1}^\dagger \times a_{j_1}^\dagger]^k \cdot [\tilde{a}_{j_1} \times \tilde{a}_{j_2}]^k .$$

From (47) we have

$$\left\langle \begin{matrix} [\bar{\nu}]\bar{\theta}J \\ \nu_1^0 J_1^0, \nu_2' J_2' \end{matrix} \middle\| V_{11,12}^k \middle\| \begin{matrix} [\nu]\theta J \\ \nu_1 J_1, \nu_2 J_2 \end{matrix} \right\rangle^{\bar{\nu}'\nu''\nu'} = \sum_{\bar{\nu}_1 \nu_1'} \langle \nu_1^0 \nu_2', \bar{\nu}\bar{\theta} | a_1^\dagger a_1^\dagger a_1 a_2 | \nu_1 \nu_2, \nu\theta \rangle_{\bar{\nu}_1 \nu_1'}^{\bar{\nu}'\nu''\nu'} \langle \nu_1^0 J_1^0 \nu_2' J_2', J \| V_{11,12}^k \| \nu_1 J_1 \nu_2 J_2, J \rangle^{\bar{\nu}_1 \nu_1'} . \quad (52)$$

Restricted to the totally antisymmetric states, from (51) we have

$$([1^{n_1+1}][1^{n_2-1}],[1^n]|a_1^\dagger a_1^\dagger a_1 a_2|[1^{n_1}][1^{n_2}],[1^n]) = (-)^{n_2-1} \frac{n_1}{n(n-1)} \sqrt{(n_1+1)n_2} . \quad (53)$$

From (52) and (53) we obtain the matrix elements for the totally antisymmetric states

$$\left[\begin{matrix} [1^n]J \\ [1^{n_1+1}]J_1^0, [1^{n_2-1}]J_2' \end{matrix} \middle\| n(n-1)[a_{j_1}^\dagger \times a_{j_1}^\dagger]^k \cdot [\tilde{a}_{j_1} \times \tilde{a}_{j_2}]^k \middle\| \begin{matrix} [1^n]J \\ [1^{n_1}]J_1, [1^{n_2}]J_2 \end{matrix} \right]$$
$$= (-)^{n_2-1} n_1 \sqrt{(n_1+1)n_2} ([1^{n_1+1}]J_1^0 [1^{n_2-1}]J_2', J \| [a_{j_1}^\dagger \times a_{j_1}^\dagger]^k \cdot [\tilde{a}_{j_1} \times \tilde{a}_{j_2}]^k \| [1^{n_1}]J_1 [1^{n_2}]J_2, J) . \quad (52')$$

Equation (52′) is identical (including the phase) to the first term of Eq. (5.74) in Ref. 9. It shows that the generalized QF is a generalization of the second QF, just as Eq. (52) is a generalization of (52′). It is worth mentioning that the derivation for the *general* expression (52) with arbitrary symmetry by the generalized QF is much simpler than the derivation for the totally antisymmetric special case by either the first QF or the second QF in Ref. 9.

VI. DISCUSSIONS

As a summary, we compare the three quantization formalisms.

The first QF. Both the state and operator have particle indices, and the operators obey the commutators,

$$[a_\alpha^\dagger(i),a_\beta^\dagger(j)]=0,\quad [a_\alpha(i),a_\beta^\dagger(j)]=\delta_{\alpha\beta}\delta_{ij}\ .$$

The first QF is most suitable for the partial space.

The second QF. Both states and operators do not have particle indices, and the operators obey either the bosonic or fermionic commutators. It works only for the total space.

The generalized QF. The states have particle indices while the operators have implied particle indices (creates or annihilates the last particle). It works for both partial and total spaces. In the totally antisymmetric (or symmetric) space, they become fermion (boson) operators. Therefore in this sense the generalized QF is a generalization of the second QF. It is superior to both the first and second QF for computing the matrix elements when each of the subspace has a definite symmetry.

The key to the present approach is the successive factorization, ever going from a larger space to a smaller space. All the formulas (22a), (23a), (24a), and (26a) have the same structure

$$\begin{aligned}(n\text{-body matrix elements in } V^{MN}) &= \sum_{(\nu)_{\rm int}} (n\text{-body matrix elements in } \mathbb{V}^{MN})_{(\nu)_{\rm int}}\\ &\quad\times\langle n\text{-body matrix elements in } V^{M}\rangle^{(\nu)_{\rm int}}\\ &\quad\times\langle n\text{-body matrix element in } V^{N}\rangle^{(\tilde\nu)_{\rm int}}\ ,\end{aligned} \tag{54a}$$

where the sum runs over the U(M) irrep labels of the intermediate states, denoted by $(\nu)_{\rm int}$. Notice that here the name "n-body operator" is used in a loose sense which includes the operators $a^\dagger$, $a^\dagger a^\dagger$, $a^\dagger a$, $a^\dagger a^\dagger aa$, etc. It is interesting to note the following. (1) The first factor in Eq. (54a) decouples the orbital space V^M from the spin space V^N; (2) In the factorization of the matrix elements for the individual space, there is no summation over the irrep labels of the intermediate states, since they have been fixed in previous factorization. It is seen that the role played by the permutation group is to provide these intermediate quantum numbers, such as ν' for the single-body operator, $\bar\nu'\nu''\nu'$ for the two-body operator, which specify the path for the factorization of the matrix elements. Therefore this formalism naturally leads to the *sum over path method*[11,13] which is crucial for large-scale shell-model calculation. (3) All these n-body matrix elements in the individual spaces can be further factorized,

$$\begin{aligned}\langle n\text{-body matrix elements in } V^{M_1+M_2}\rangle^{(\nu)_{\rm int}} &= \sum_{(\nu_1\nu_2)_{\rm int}} \langle n\text{-body matrix elements in } \mathbb{V}^{M_1+M_2}\rangle^{(\nu)_{\rm int}}_{(\nu_1\nu_2)_{\rm int}}\\ &\quad\times[\text{SO(3) coupling coeff.}]\langle \mathfrak{m}_1\text{-operator matrix elements in } V^{M_1}\rangle^{(\nu_1)_{\rm int}}\\ &\quad\times\langle \mathfrak{m}_2\text{-operator matrix elements } V^{M_2}\rangle^{(\nu_2)_{\rm int}}\ ,\end{aligned} \tag{54b}$$

$$\begin{aligned}\langle n\text{-body matrix elements in } V^{N_1N_2}\rangle^{(\tilde\nu)_{\rm int}} &= \sum_{(\nu_s\nu_t)_{\rm int}} \langle n\text{-body matrix elements in } \mathbb{V}^{N_1N_2}\rangle^{(\tilde\nu)_{\rm int}}_{(\nu_s\nu_t)_{\rm int}}\\ &\quad\times(n\text{-body matrix elements in } V^{N_1})^{(\nu_s)_{\rm int}}(n\text{-body matrix elements in } V^{N_2})^{(\nu_s)_{\rm int}}\ ,\end{aligned} \tag{54c}$$

where it is assumed that there are $\mathfrak{m}_1$ and $\mathfrak{m}_2$ creation or/and annihilation operators belonging to shell 1 and shell 2, respectively, in the n-body operator.

The factorization (54b) and (54c) is of paramount importance in the development of a multishell, multispin code, since we now only need to store the single-shell matrix elements ($\mathfrak{m}_i$-operator matrix elements in V^{M_i}) and single-spin matrix elements (n-body matrix elements in V^{N_i}).

The second QF works only for the totally antisymmetric (or symmetric) states in the space V^{MN} (or $V^{M_1+M_2}$), while the generalized QF works for the space V^{MN} (or $V^{M_1+M_2}$) with arbitrary symmetry including totally antisymmetric or symmetric cases as two special cases.

The advantages of the present approach over the CFP technique are that (1) the one- or two-body operators are often expressed in the second QF. With the generalized QF, we are spared the inconvenience of having to switch back to the first QF for computing their matrix elements. (2) In this approach, we focus our attention solely on the reduced matrix elements without using any wave functions and the irreducible tensor technique can be utilized in a straightforward way.

ACKNOWLEDGMENTS

The author is very grateful to A. Novoselsky, M. Vallieres, R. Gilmore, D. H. Feng, K. T. Hecht, and Bing-Qing Chen for numerous discussions. This work was supported by the U.S. National Science Foundation and Chinese Science Foundation.

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