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Young invariant decomposition of spin-interacting operators

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Abstract. The Young invariant decomposition of totally symmetric spin-interacting operators is examined from the viewpoint of outer-product isoscalar factors of the symmetric group. The coefficients required for the decomposition of one- and two-body operators are constructed and given explicitly. The formalism enables a separate treatment of the spatial and spin parts of the matrix elements of the spin-interacting operators.

1. Introduction

Many operators of physical significance depend on more than two parts of the intrinsic space of many-body systems. Familiar examples are spin-interacting operators in atomic and molecular physics, for which the total Hamiltonian can be written as the product of operators that are acting only on the spatial and spin spaces, respectively. Such operators are of importance when investigating the relativistic effects of systems containing heavy atoms. A similar type of operators can be found in nuclear physics. Recently the use of group-theoretical techniques for the calculation of the matrix elements of the spin-dependent operators in atomic and molecular physics has attracted great attention (Gould and Chandler 1984, Gould and Paldus 1990, Gould and Battle 1993). In a recent paper (Zhang and Li 1989), the matrix-element calculation of the spin-interacting operators was examined from the viewpoint of the permutation group technique, based on an early investigation of Cooper and Musher (1972, 1973) and some new developments in the representation theory of the permutation group (Chen 1989, Li 1989, Li and Zhang 1987, 1989a, Li and Paldus 1989, 1990, 1993, Zhang and Li 1986, 1987). The method is an irreducible tensor operator calculus based on the symmetric group (S_N) representation theory.

Various kinds of spin-interacting operators can be found in physics and quantum chemical many-body problems. Consider, for specificity, a class of operators which satisfy or can be transformed into the following form:

$$\hat{H} = \sum_{\omega} \hat{h}_r(\omega)\hat{h}_\sigma(\omega) \tag{1}$$

where $\hat{h}_r$ and $\hat{h}_\sigma$ are defined separately in the spatial (r) and spin (σ) spaces, $\omega = i$ for one-body operators and $\omega = (i, j)$ for two-body operators. The operator $\hat{H}$ is totally symmetric with respect to a simultaneous permutation of the spatial and spin coordinates of particles but does not possess any symmetry with respect to the individual permutation of the spatial or spin coordinates. However, a formulation with higher symmetry can be achieved since we can rewrite the operator (1) as

$$\hat{H} = \sum_{[\mu]k} \hat{h}_{r}^{[\mu]k} \hat{h}_{\sigma}^{[\mu]k} \tag{2}$$

where $\hat{h}_{r}^{[\mu]k}$ ($\hat{h}_{\sigma}^{[\mu]k}$ similarly) transforms as an irreducible basis of S_N (the permutation group of N identical particles), denoted by the Young tableau $Y^{[\mu]k}$ (i.e. the kth tableau of the Young diagram $[\mu]$). Such a procedure is referred to as a Young invariant decomposition of the spin-interacting operator, since with respect to the separate permutations on the spatial or spin coordinates the operators $\hat{h}_{r}^{[\mu]k}$ and $\hat{h}_{\sigma}^{[\mu]k}$ in (2) transform within a given irreducible representation (irrep) space characterized by a Young diagram $[\mu]$. The decomposition will facilitate the treatment of the matrix elements of $\hat{H}$ using the group tensorial algebra. This consideration is motivated by the widely-used approach to the construction of the molecular electronic wavefunction through the expansion in terms of spin-free states, such as the Gelfand–Tsetlin bases in the unitary group approach (Paldus 1974, 1976, Paldus and Boyle 1980, Shavitt 1977, 1978, Hinze 1981, Matsen and Pauncz 1986) or chemically more interesting valence band-type bases (Paldus and Sarma 1985, Li and Zhang 1989b). It is thus desirable that one can calculate the relativistic effects directly and separately from the spatial and spin functions, avoiding the coupling of the spin-free states with spin functions in order to obtain totally antisymmetric states. Equation (2) represents just such a fundamental problem existing in the symmetric group approach (see Zhang and Li (1989)).

It has been proved that the Young invariant decomposition of the spin-interacting operators is closed in relation to the so-called outer-product coupling scheme of S_N. In fact the operators in (2) are linear combinations of the operators in (1) with the linear combination coefficients being equal to the outer-product coupling coefficients (OPCC) (Li and Zhang 1989a, Zhang and Li 1987, Li and Paldus 1990). From group representation theory, it is well known that all these coupling coefficients can be factorized into successive products of isoscalar factors which depend only on group–subgroup properties, a generalization of Racah's factorization lemma (Racah 1965) to the symmetric group. In our case, the outer-product isoscalar factors of S_N are required.

In this article we derive all the required outer-product isoscalar factors for one- and two-body spin-interacting operators. From these isoscalar factors the Young invariant decomposition of the one- and two-body operators are given explicitly. After a brief discussion of the basic formalism, the essential isoscalar factors are derived in section 2. In section 3, we present explicit expressions for the linear combinations which determine the decomposition. A discussion is given in section 4.

2. Isoscalar factors

Consider one- and two-body spin-interacting operators

$$\hat{H} = \sum_{i} \hat{a}(r_i)\hat{b}(\sigma_i) \tag{3}$$

$$\hat{H}' = \sum_{i<j} \hat{f}(r_i, r_j)\ \hat{g}(\sigma_i, \sigma_j) \tag{4}$$

where $\hat{a}$ and $\hat{f}$ are operators acting on the spatial space, while $\hat{b}$ and $\hat{g}$ act on the spin space. Clearly the spin–orbit coupling is of the form (3). For the two-body operator, (4), we could further distinguish between the symmetric and antisymmetric two-body operators, by which we mean that the operators $\hat{f}$ and $\hat{g}$ which satisfy

$$\hat{f}_{\mathrm{S}}(\boldsymbol{r}_i, \boldsymbol{r}_j) = \hat{f}_{\mathrm{S}}(\boldsymbol{r}_j, \boldsymbol{r}_i) \qquad \hat{g}_{\mathrm{S}}(\sigma_i, \sigma_j) = \hat{g}_{\mathrm{S}}(\sigma_j, \sigma_i) \tag{5}$$

or

$$\hat{f}_{\mathrm{A}}(\boldsymbol{r}_i, \boldsymbol{r}_j) = -\hat{f}_{\mathrm{A}}(\boldsymbol{r}_j, \boldsymbol{r}_i) \qquad \hat{g}_{\mathrm{A}}(\sigma_i, \sigma_j) = -\hat{g}_{\mathrm{A}}(\sigma_j, \sigma_i). \tag{6}$$

Even though the original two-body operators may not have such a symmetry property, their symmetric and antisymmetric components can be constructed in such a way that we always assume that (5) and (6) are satisfied. We can thus write

$$\hat{H}' = \hat{H}'_{\mathrm{S}} + \hat{H}'_{\mathrm{A}} \tag{7}$$

where

$$\hat{H}'_{\Gamma} = \sum_{i<j} \hat{f}_{\Gamma}(\boldsymbol{r}_i, \boldsymbol{r}_j)\hat{g}_{\Gamma}(\sigma_i, \sigma_j) \qquad (\Gamma = \mathrm{S}, \mathrm{A}). \tag{8}$$

We now consider the Young invariant decomposition of the operators (3) and (8). The linear combinations of one- or two-body operators will form the irreducible bases for the permutation group S_N. It has been proved (Zhang and Li 1989) that the linear combination coefficients are the so-called OPCC of S_N. Explicitly, we have the following results for the one-body operators:

$$\hat{H} = \sum_{[\mu]k} \hat{a}^{[\mu]k}\hat{b}^{[\mu]k} \tag{9}$$

where the operators $\hat{a}^{[\mu]k}$ and $\hat{b}^{[\mu]k}$ are linear combinations of the operators $\hat{a}$ and $\hat{b}$, respectively. For example, we have

$$\hat{a}^{[\mu]k} = \sum_i c_i^{[\mu]k}\hat{a}(\boldsymbol{r}_i) \tag{10}$$

where $c_i^{[\mu]k}$ is an OPCC given by

$$c_i^{[\mu]k} = \left(\begin{array}{cc|c} [N-1] & [1] & [\mu] \\ 1(\omega) & 1(i) & k \end{array} \right). \tag{11}$$

The same coefficients $c_i^{[\mu]k}$ can be used to construct $b^{[\mu]k}$ from b. In (11), the Young tableaux are given by

$$|[1]1(i)\rangle = \boxed{i} \tag{12}$$

and

$$|[N-1]1(\omega)\rangle = \begin{array}{|c|c|c|c|c|c|}\hline 1 & \cdots & i_1 & i_2 & \cdots & N \\ \hline \end{array} \tag{13}$$

where $i_1 = i - 1$, $i_2 = i + 1$ and ω is the index set consisting of $1, 2, \ldots, N$ but do not include i. $|[\mu]k\rangle$ is the resulting Young tableau from the coupling of the bases for $[1]$ and $[N-1]$. The possible Young diagrams $[\mu]$s are determined by the Littlewood rule, which is the branch rule for the outer-product reduction. It is easily found that $[\mu]$ can be either $[N]$ or $[N-1, 1]$. The corresponding Young tableaux are $|[N]1\rangle$ and $|[N-1, 1]r\rangle$, where

$$|[N-1, 1]\, r\rangle \;=\; \begin{array}{|c|c|}\hline 1 & \cdots \\ \hline k & \\ \cline{1-1} \end{array} \tag{14}$$

with $k = 2, 3, \ldots, N$ and $r = k - 1$ being the Young–Yamanouchi index.

For the two-body operators, the situation is completely similar. For the symmetric operators, $\hat{H}'_{\mathrm{S}}$, we have

$$\hat{H}'_{\mathrm{S}} = \sum_{[\mu]k} \hat{f}_{\mathrm{S}}^{[\mu]k} \hat{g}_{\mathrm{S}}^{[\mu]k} \tag{15}$$

$$\hat{h}_{\mathrm{S}}^{[\mu]k} = \sum_{i<j} c_{\mathrm{S},ij}^{[\mu]k} \hat{h}_{\mathrm{S}}(\boldsymbol{r}_i, \boldsymbol{r}_j) \qquad (h = f, g). \tag{16}$$

Here the coefficient $c_{\mathrm{S},ij}^{[\mu]k}$ is an OPCC given by

$$c_{\mathrm{S},ij}^{[\mu]k} = \left(\begin{array}{cc|c} [N-2] & [2] & [\mu] \\ 1(\omega) & 1(ij) & k \end{array} \right) \tag{17}$$

where $[\mu] = [N], [N-1, 1], [N-2, 2]$ is determined by the Littlewood rule. Similarly, for the antisymmetric operators $\hat{H}'_{\mathrm{A}}$, we get

$$\hat{H}'_{\mathrm{A}} = \sum_{[\mu]k} \hat{f}_{\mathrm{A}}^{[\mu]k} \ \hat{g}_{\mathrm{A}}^{[\mu]k} \tag{18}$$

$$\hat{h}_{\mathrm{A}}^{[\mu]k} = \sum_{i<j} c_{\mathrm{A},ij}^{[\mu]k} \hat{h}_{\mathrm{A}}(\boldsymbol{r}_i, \boldsymbol{r}_j) \qquad (h = f, g) \tag{19}$$

with the linear combination coefficients being the OPCCs

$$c_{\mathrm{A},ij}^{[\mu]k} = \left(\begin{array}{cc|c} [N-2] & [1^2] & [\mu] \\ 1(\omega) & 1(ij) & k \end{array} \right). \tag{20}$$

Again, $[\mu] = [N-1, 1], [N-2, 1^2]$, given by the Littlewood rule. In (17) and (20), the Young tableaux are schematically given by

$$|[2]1(ij)\rangle = \begin{array}{|c|c|}\hline i & j \\ \hline \end{array} \tag{21}$$

$$|[1^2]1(ij)\rangle = \begin{array}{|c|}\hline i \\ \hline j \\ \hline \end{array} \tag{22}$$

$$|[N-2]1(\omega)\rangle = \begin{array}{|c|c|c|}\hline 1 & \cdots & N \\ \hline \end{array} \tag{23}$$

where the last Young tableau contains all indices in ω which consists of 1, 2, …, N but do not include i and j. The possible resulting Young tableaux for irreps $[N-2, 2]$ and $[N-2, 1^2]$ are given as follows.

$$|[N-2, 2]\ s\rangle = \begin{array}{|c|c|c}\hline 1 & \cdot\cdot & \multicolumn{1}{c|}{\cdots} \\ \hline k & l & \\ \cline{1-2} \end{array} \tag{24}$$

$$|[N-2, 1^2]\ t\rangle = \begin{array}{|c|c}\hline 1 & \multicolumn{1}{c|}{\cdots} \\ \hline k & \\ \cline{1-1} l & \\ \cline{1-1} \end{array} \tag{25}$$

Once the actual values of k and l are given, the Young–Yamanouchi indices s and t are uniquely determined.

The OPCCs appearing in (11), (17) and (20) can be expressed as successive products of outer-product isoscalar factors (Zhang and Li 1987, Li and Zhang 1989a) (I_{o} factors for short). All required I_{o} factors in our cases are given in table 1. Here we briefly give their derivation. For the sake of simplicity, only the case numbers are indicated.

Table 1. Outer-product isoscalar factors, $I_0\left(\begin{array}{cc|c} [\lambda] & [\mu] & [\nu] \\ [\lambda'] & [\mu'] & [\nu'] \end{array}\right)$, required for the construction of irreducible bases of S_N from the linear combinations of one- and two-body operators.

Cases	$[\lambda]$	$[\mu]$	$[\nu]$	$[\lambda']$	$[\mu']$	$[\nu']$	I_0
1	$[N-1]$	$[1]$	$[N]$	$[N-1]$	$[0]$	$[N-1]$	$N^{-1/2}$
2				$[N-2]$	$[1]$	$[N-1]$	$[(N-1)/N]^{1/2}$
3	$[N-1]$	$[1]$	$[N-1,1]$	$[N-1]$	$[0]$	$[N-1]$	$[(N-1)/N]^{1/2}$
4				$[N-2]$	$[1]$	$[N-1]$	$-N^{-1/2}$
5				$[N-2]$	$[1]$	$[N-2,1]$	1
6	$[N-2]$	$[2]$	$[N]$	$[N-2]$	$[1]$	$[N-1]$	$(2/N)^{1/2}$
7				$[N-3]$	$[2]$	$[N-1]$	$[(N-2)/N]^{1/2}$
8	$[N-2]$	$[2]$	$[N-1,1]$	$[N-2]$	$[1]$	$[N-1]$	$[(N-2)/N]^{1/2}$
9				$[N-2]$	$[1]$	$[N-2,1]$	$(N-2)^{-1/2}$
10				$[N-3]$	$[2]$	$[N-1]$	$-(2/N)^{1/2}$
11				$[N-3]$	$[2]$	$[N-2,1]$	$[(N-3)/(N-2)]^{1/2}$
12	$[N-2]$	$[2]$	$[N-2,2]$	$[N-2]$	$[1]$	$[N-2,1]$	$[(N-3)/(N-2)]^{1/2}$
13				$[N-3]$	$[2]$	$[N-2,1]$	$-(N-2)^{-1/2}$
14				$[N-3]$	$[2]$	$[N-3,2]$	1
15	$[N-2]$	$[1^2]$	$[N-1,1]$	$[N-2]$	$[1]$	$[N-1]$	1
16				$[N-2]$	$[1]$	$[N-2,1]$	$-N^{-1/2}$
17				$[N-3]$	$[1^2]$	$[N-2,1]$	$[(N-1)/N]^{1/2}$
18	$[N-2]$	$[1^2]$	$[N-2,1^2]$	$[N-2]$	$[1]$	$[N-2,1]$	$[(N-1)/N]^{1/2}$
19				$[N-3]$	$[1^2]$	$[N-2,1]$	$N^{-1/2}$
20				$[N-3]$	$[1^2]$	$[N-1]$	1

Cases 1 and 3 can be directly obtained by using a closed formula (Zhang and Li 1987), namely,

$$I_0\left(\begin{array}{cc|c} [\lambda] & [1] & [\nu] \\ [\lambda] & 0 & [\lambda] \end{array}\right) = \left(\frac{f_{[\nu]}}{Nf_{[\lambda]}}\right)^{1/2} \tag{26}$$

where $f_{[\nu]}$ is the dimension of $[\nu]$ and N is the particle number. To determine the cases of 2 and 4, we applied the normalization condition to give

$$I_0\left(\begin{array}{cc|c} [N-1] & [1] & [N] \\ [N-2] & [1] & [N-1] \end{array}\right) = \pm\left(\frac{N-1}{N}\right)^{1/2} \tag{27}$$

$$I_0\left(\begin{array}{cc|c} [N-1] & [1] & [N-1,1] \\ [N-2] & [1] & [N-1] \end{array}\right) = \pm N^{-1/2}. \tag{28}$$

Using the symmetry relation of the I_0 factor (Li 1989), we find

$$I_0\left(\begin{array}{cc|c} [N-1] & [1] & [N] \\ [N-2] & [1] & [N-1] \end{array}\right) = I_0\left(\begin{array}{cc|c} [1] & [N-1] & [N] \\ [1] & [N-2] & [N-1] \end{array}\right). \tag{29}$$

In accordance with the extended Condon–Shortley phase convention (Zhang and Li 1987), the factor on the right-hand side is positive. Hence (27) is positive. Similarly, we find

$$\begin{aligned} I_0 &\left(\begin{array}{cc|c} [N-1] & [1] & [N-1,1] \\ [N-2] & [1] & [N-1] \end{array} \right) \\ &= (-1)^{[N-2]+[N-1,1]} I_0 \left(\begin{array}{cc|c} [1] & [N-1] & [N-1,1] \\ [1] & [N-2] & [N-1] \end{array} \right) = -N^{-1/2} \end{aligned} \tag{30}$$

since $(-1)^{[N-1,1]} = -1$ and the I_0 factor on the right-hand side of (30) is positive by the convention. Case 5 is a direct result of the normalization.

For irreps $[\mu] = [2]$ and $[1^2]$, we have derived the following compact expressions (Zhang and Li 1987):

$$I_0 \left(\begin{array}{cc|c} [\lambda_1] & [\lambda_2] & [\lambda] \\ [\lambda_1] & [1] & [\lambda-1, \rho_N^2] \end{array} \right) = \left(\frac{(\tau + \delta_{[\lambda_2]}) f_{[\lambda]}}{N \ \tau \ f_{[\lambda-1, \rho_N^2]}} \right)^{1/2} \tag{31}$$

$$I_0 \left(\begin{array}{cc|c} [\lambda_1] & [\lambda_2] & [\lambda] \\ [\lambda_1] & [1] & [\lambda-1, \eta_N^2] \end{array} \right) = \delta_{[\lambda_2]} \left(\frac{(\tau - \delta_{[\lambda_2]}) f_{[\lambda]}}{N \ \tau \ f_{[\lambda-1, \eta_N^2]}} \right)^{1/2} \tag{32}$$

where $[\lambda_2] = [2]$ ($\delta_{[2]} = 1$) or $[\lambda_2] = [1^2]$ ($\delta_{[1^2]} = -1$). The irrep $[\lambda]$ is obtained by adding two boxes to $[\lambda_1]$. Assuming that the row indices of these two added boxes are η_N^2 and ρ_N^2 ($\eta_N^2 \leqslant \rho_N^2$), respectively, then the τ is the axis distance from the box η_N^2 to box ρ_N^2. The irrep $[\lambda-1, \rho_N^2]$ is obtained from $[\lambda]$ by removing the box ρ_N^2 (or, equivalently, obtained from $[\lambda_1]$ by adding one box to row η_N^2). Equations (31) and (32) can be used to derive the formulae for the cases 6, 8, 9, 12, 15, 16 and 18. For example, for case 16, we have

$$I_0 \left(\begin{array}{cc|c} [N-2] & [1^2] & [N-1,1] \\ [N-2] & [1] & [N-2,1] \end{array} \right) = - \left[\frac{(-N) f_{[N-1,1]}}{N(-N+1) f_{[N-2,1]}} \right]^{1/2} . \tag{33}$$

Similar calculations can be done for cases 6, 8, 9, 12, 15 and 18. From these calculated I_0 factors and employing the symmetry property (Li, 1989), cases 7, 10, 13, 17 and 19 are then subsequently determined. Case 11 is slightly special. Its absolute value can easily be determined while its phase requires a consideration, because we cannot fix the phase of

$$I_0 \left(\begin{array}{cc|c} [2] & [N-2] & [N-1,1] \\ [2] & [N-3] & [N-2,1] \end{array} \right) \tag{34}$$

from the phase convention. Exploiting the recursive formula (23) from Zhang and Li (1987), we find

$$\begin{aligned} &\operatorname{sgn} I_0 \left(\begin{array}{cc|c} [2] & [N-2] & [N-1,1] \\ [2] & [N-3] & [N-2,1] \end{array} \right) \times \operatorname{sgn} I_0 \left(\begin{array}{cc|c} [2] & [N-2] & [N-1,1] \\ [2] & [N-3] & [N-1] \end{array} \right) \\ &\quad = \operatorname{sgn} I_0 \left(\begin{array}{cc|c} [2] & [N-3] & [N-2,1] \\ [2] & [N-4] & [N-2] \end{array} \right) \\ &\quad \times \operatorname{sgn} I_0 \left(\begin{array}{cc|c} [2] & [N-3] & [N-1] \\ [2] & [N-4] & [N-2] \end{array} \right). \end{aligned} \tag{35}$$

All I_0 factors except the first one on the left-hand side are known to be positive. This means that (34) is positive as is case 11. Finally, cases 14 and 20 are obtained from the normalization.

3. Explicit coefficients determining Young invariant decomposition

The I_o factors given in table 1 play an essential role in constructing the OPCCs required for the Young invariant decomposition of spin-coupled operators. Based on table 1, it is straightforward to derive the explicit expressions for the necessary coefficients in (11), (17) and (20).

Consider, for example, the coefficient $C_{S,ij}^{[N-2,2]s}$ of (17) with the Young tableau $|[\mu]k\rangle = |[N-2,2]s\rangle$, (24), and $i = k < j < l$. This coefficient is an OPCC, in accordance with (17) and can thus be calculated as a successive product of I_o factors from level N to level 1. The following formulae are required for the levels indicated in the parentheses:

$$I_o\left(\begin{array}{cc|c} [M-2] & [2] & [M-2,2] \\ [M-3] & [2] & [M-3,2] \end{array}\right) = 1 \qquad (l+1 \leqslant M \leqslant N) \tag{36}$$

$$I_o\left(\begin{array}{cc|c} [l-2] & [2] & [l-2,2] \\ [l-3] & [2] & [l-2,1] \end{array}\right) = -\,(l-2)^{-1/2} \qquad \text{(at level } l) \tag{37}$$

$$I_o\left(\begin{array}{cc|c} [M-2] & [2] & [M-1,1] \\ [M-3] & [2] & [M-2,1] \end{array}\right) = \left(\frac{M-3}{M-2}\right)^{1/2} \qquad (j+1 \leqslant M \leqslant l-1) \tag{38}$$

$$I_o\left(\begin{array}{cc|c} [j-2] & [2] & [j-1,1] \\ [j-2] & [1] & [j-2,1] \end{array}\right) = (j-2)^{-1/2} \qquad \text{(at level } j) \tag{39}$$

$$I_o\left(\begin{array}{cc|c} [M-1] & [1] & [M-1,1] \\ [M-2] & [1] & [M-2,1] \end{array}\right) = 1 \qquad (k+1 \leqslant M \leqslant j-1) \tag{40}$$

$$I_o\left(\begin{array}{cc|c} [k-1] & [1] & [k-1,1] \\ [k-1] & [0] & [k-1] \end{array}\right) = \left(\frac{k-1}{k}\right)^{1/2} \qquad \text{(at level } i = k) \tag{41}$$

while $I_o = 1$ under level i. From the above isoscalar factors, we have

$$C_{S,ij}^{[N-2,2]s} = -\left[\frac{(k-1)}{k(l-3)(l-2)}\right]^{1/2}. \tag{42}$$

This procedure can easily be applied to other coefficients. Thus, all the necessary coefficients have been determined and summarized as follows.

(i) $c_i^{[\mu]k}$ for the one-body operators. There are two possible symmetry patterns, $[\mu] = [N]$ and $[N-1,1]$. The corresponding coefficients are given as follows

$$C_i^{[N]1} = N^{-1/2} \tag{43}$$

and

$$C_i^{[N-1,1]r} = \begin{cases} -[(k-1)k]^{-1/2} & (i < k) \\ [(k-1)/k]^{1/2} & (i = k) \\ 0 & (i > k) \end{cases} \tag{44}$$

where k is given by the basis $|[N-1,1]r\rangle$, (14).

(ii) $c_{S,ij}^{[\mu]k}$ for the symmetric two-body operators. Corresponding to $[\mu] = [N]$, $[N-1,1]$, $[N-2,2]$ we have

$$C_{S,ij}^{[N]1} = [2/(N-1)N]^{1/2} \tag{45}$$

$$C_{S,ij}^{[N-1,1]r} = \begin{cases} 0 & (k < i < j) \\ -2x & (i < j < k) \\ (k-2)x & (i < j = k) \\ -x & (i < k < j) \\ (k-1)x & (i = k < j) \end{cases} \tag{46}$$

where k is given by the basis $|[N-1,1]r\rangle$, (14) and

$$x = [(k-1)k(N-2)]^{-1/2}. \tag{47}$$

Finally,

$$C_{S,ij}^{[N-2,2]s} = \begin{cases} 0 & (j > l \text{ or } k < i < j \leqslant l) \\ 2y & (i < j < k < l) \\ -(k-2)y & (i < j = k < l) \\ y & (i < k < j < l) \\ -(k-1)y & (i = k < j < l) \\ (l-3)y & (i < k < j = l) \\ (k-1)(l-3)y & (i = k < j = l) \end{cases} \tag{48}$$

where k and l are given by the basis $|[N-2,2]s\rangle$, (24), and

$$y = [(k-1)k(l-3)(l-2)]^{-1/2}. \tag{49}$$

(iii) $c_{A,ij}^{[\mu]k}$ for the antisymmetric two-body operators. For $[\mu] = [N-1,1]$ we have

$$C_{A,ij}^{[N-1,1]r} = \begin{cases} 0 & (i < j < k \text{ or } k < i < j) \\ [k/(k-1)N]^{1/2} & (i < j = k) \\ [(k-1)kN]^{-1/2} & (i < k < j) \\ -[(k-1)/kN]^{1/2} & (i = k < j) \end{cases} \tag{50}$$

where k is given by the basis $|[N-1,1]r\rangle$. For $[\mu] = [N-2,1^2]$ we get

$$C_{A,ij}^{[N-2,1^2]t} = \begin{cases} 0 & (j > l, \text{ or } i < j < k < l \text{ or } k < i < j \leqslant l) \\ kz & (i < j = k < l) \\ -(k-1)z & (i = k < j < l) \\ z & (i < k < j < l) \\ -(l-1)z & (i < k < j = l) \\ (k-1)(l-1)z & (i = k < j = l) \end{cases} \tag{51}$$

where k and l are given by the basis $|[N-2,1^2]t\rangle$, (25), and

$$z = [(k-1)k(l-1)l]^{-1/2}. \tag{52}$$

It is noted that all the symmetry adapted coefficients are square roots of simple rational numbers and depend on the particle indices i, j and the key indices k and/or l which characterized the Young tableaux (14), (24) and (25). Moreover, these coefficients satisfy the following orthogonality relations:

$$\sum_{\omega} C_{\omega}^{[\mu]s} C_{\omega}^{[\nu]t} = \delta_{\mu\nu}\delta_{st} \tag{53}$$

$$\sum_{\mu,s} C_{\omega}^{[\mu]s} C_{\omega'}^{[\mu]s} = \delta_{\omega\omega'} \tag{54}$$

where $\omega = (i)$ and (i,j) for one- and two-body operators, respectively.

4. Discussion

The Young invariant decomposition of the spin-interacting operators provides the possibility that the matrix elements can be factorized into a product of the spatial and spin parts, which simplifies the computation and is desirable when the zero-order wavefunction is calculated from the expansion of spin-free bases. As is well known, the total wavefunction can be written as the coupling of the spatial and spin functions

$$\Psi = f_{[\lambda]}^{-1/2} \sum_r \Lambda_r^{[\lambda]} \Phi_r^{[\lambda]} \Theta_{\bar{r}}^{[\tilde{\lambda}]} \tag{55}$$

where $\Phi_r^{[\lambda]}$ is the spatial function belonging to the rth component of the irrep $[\lambda]$, $\Theta_{\bar{r}}^{[\tilde{\lambda}]}$ is the corresponding conjugated spin function and $\Lambda_r^{[\lambda]}$ is the coupling coefficient. The matrix elements of these states for the operator (2) can then be expressed in a compact formalism as the products of reduced matrix elements on the spatial and spin spaces (Zhang and Li 1989)

$$\langle\Psi|\hat{H}|\Psi'\rangle = (f_{[\lambda]} f_{[\nu]})^{-1/2} \sum_{\mu} \left\langle \Phi^{[\lambda]} \left\| \hat{h}_r^{[\mu]} \right\| \Phi^{[\nu]} \right\rangle \left\langle \Theta^{[\tilde{\lambda}]} \left\| \hat{h}_\sigma^{[\mu]} \right\| \Theta^{[\tilde{\nu}]} \right\rangle \tag{56}$$

employing the Wigner–Eckart theorem. Here the reduced matrix element is defined by, e.g.,

$$\left\langle \Phi^{[\lambda]} \left\| \hat{h}_r^{[\mu]} \right\| \Phi^{[\nu]} \right\rangle = \left\langle \Phi_r^{[\lambda]} \left| \hat{h}_r^{[\mu]s} \right| \Phi_t^{[\nu]} \right\rangle \left(\begin{array}{cc|c} [\lambda] & [\mu] & [\nu] \\ r & s & t \end{array} \right)^{-1} \tag{57}$$

with the last factor being a Clebsch–Gordan coefficient (or the so-called inner-product coupling coefficient) for the permutation group (cf, e.g., Chen 1989, Zhang and Li 1986, 1987). A similar expression can be written for the reduced matrix elements on the spin space. It is clear that the Young invariant decomposition leads to a simpler formalism of the matrix element evaluation, from which we can analysis the significance of the contribution from the different spaces and gain an insight into the structure of the relevant matrix.

It is noted that the coefficients determining the decomposition are universal and applicable to any many-body systems. The Young invariant decomposition for the operators that depends on more than two parts of intrinsic spaces can be carried out in a similar way. For example, a one-body operator depending on three spaces can be decomposed as

$$\hat{H} = \sum_i \hat{a}(r_i)\hat{b}(\sigma_i)\hat{c}(\tau_i) = \sum_{\lambda r} \sum_{\mu s} \sum_{\nu t} \hat{a}_r^{[\lambda]} \hat{b}_s^{[\mu]} \hat{c}_t^{[\nu]} \tag{58}$$

where the sum is over all possible irreps which could give $[\lambda] \times [\mu] \times [\nu] \supset [N]$. In the case of a one-body operator, we have

$$\begin{aligned} \hat{H} = \hat{a}_1^{[N]} \hat{b}_1^{[N]} \hat{c}_1^{[N]} + \hat{a}_1^{[N]} \sum_r \hat{b}_r^{[N-1,1]} \hat{c}_r^{[N-1,1]} \\ + \hat{b}_1^{[N]} \sum_r \hat{a}_r^{[N-1,1]} \hat{c}_r^{[N-1,1]} + \hat{c}_1^{[N]} \sum_r \hat{a}_r^{[N-1,1]} \hat{b}_r^{[N-1,1]}. \end{aligned} \tag{59}$$

The factorization of the matrix elements can then be proceeded similarly.

The present discussion on the structure of matrix elements employs the permutation group representation theory and uses the outer-product coupling coefficients for the symmetry adaptation of the relevant operators. In view of the fact that there is a close relationship between the symmetric and unitary group representation, it is believed that the combination of the present symmetric group formalism with the versatile unitary group approach will yield a more efficient method for matrix-element evaluation.

Finally, we should also add that there is a duality between the outer-product coupling coefficient of the permutation group S_N and the inner-product coupling coefficients (i.e. Clebsch–Gordan (CG) coefficients) of the unitary group $U(n)$. This duality has been extensively employed for the evaluations of the CG coefficients of $U(n)$ (see, e.g., Chen 1987, Chen *et al* 1989, Zhang and Li 1987, Li and Paldus 1990). The distinguishing feature of the permutation group approach to the $U(n)$ CG coefficient problem is that the resulting CG coefficients (or, in fact, the corresponding isoscalar factors) are n-independent (but depend on N, the number of particles). This allows the computations of the $U(n)$ CG coefficients (or isoscalar factors) for arbitrary n. For the few-body problem (N up to 6), all possible outer-product isoscalar factors for S_6 have been computed and tabulated (Chen *et al* 1987), which can be used to evaluated $U(n)$ CG coefficients for up to six-body problems. Since we are interested in general many-electron problems, for which the number of electrons could be fairly large, it is important to derive all the required coefficients in closed formulae, which is very difficult for general irreducible representations. However, for certain classes of problems which interest us, this goal can be achieved (Li and Paldus 1989, 1990). The present article thus demonstrates another such case for the Young invariant decomposition of spin-interacting operators.

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