

## A Programmable Spin-Free Method for Configuration Interaction

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In this note a method is presented for quick implementation of configuration interaction (CI) calculations in molecules. A spin-free Hamiltonian for an  $N$  electron system in a spin state  $S$ , expressed in terms of the generators for the unitary group algebra, is diagonalized over orbital configurations forming a basis for the irreducible representation  $[2^{1/2N-S}1^{2S}]$  of the permutation group  $S_N$ . It has been found that the basic algebraic expressions necessary for the CI calculation involve a limited category of permutations. These have been displayed explicitly.

**Key words:** Configuration interaction

### 1. Introduction

In recent years extensive investigations have been undertaken in Configuration Interaction (CI) studies of molecules using permutation and unitary group algebras [1-9]. Two of these are mainly computation oriented [1, 9]. The former [1] leads to compact expressions for the CI matrix elements of a spin-free Hamiltonian in terms of the Irreducible Representation (IR) matrices of the permutation group  $S_N$ . Ten basic expressions are provided from which any required CI matrix element can be evaluated. The only difficulty in using this approach for computations is that the "matching" permutations have not been explicitly obtained and are difficult to handle. Further, the ordering of the orbitals entering a given configuration is not the conventional one.

The second approach [9] is based on the unitary group algebra and diagonalizes a model spin-free Hamiltonian over the Gelfand-Zetlin basis [4-6, 9, 10]. The

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computational methods involved in handling large systems using this approach are still in the process of development.

In the present note an attempt has been made to combine the algebra of the Young idempotents of the permutation group with a model Hamiltonian expressed in terms of the generators of the unitary group algebra to obtain a basic category of expressions for the CI matrix elements. This procedure is found to lead to explicit forms for the matching permutations and enables easier programming. The method is developed in Sect. 2, and the results obtained are summarized in the Appendix. In Sect. 3 a brief discussion of the method is presented.

## 2. The Present Approach

Consider an  $N$ -electron system whose interactions are described by a spin-free Hamiltonian. Assume that a set of  $M$  orthonormal spatial one-electron orbitals have been provided, which span a linear space  $v_M^r$ ,

$$v_M^r: \{\phi_i(r) | i=1, \dots, M\} \quad (1)$$

The symmetry group on the space is the unitary group  $U_M$ , whose elements define the mapping  $v_M^r \rightarrow v_M^r$ .

The spin-free part of the  $N$ -electron function is then realized as a tensorial product forming a basis for  $v_M^r \otimes^N$

$$v_M^r \otimes^N: \{\Phi_{(i)} \equiv \Phi_{i_1 i_2 \dots i_N} | i_1 i_2 \dots i_N = 1, \dots, M\} \quad (2)$$

where

$$\Phi_{(i)} = \prod_{\mu=1}^N \otimes \phi_{i_\mu}(r_\mu). \quad (3)$$

The space  $v_M^r \otimes^N$  is decomposable into the non-equivalent IR's  $[\lambda]$  of  $S_N$ , the permutation group, on the electron coordinates. The (normalized) Young idempotents providing the decomposition are [2, 3, 11, 12]

$$\omega_{\rho'\rho}^\lambda = \left(\frac{f_N^\lambda}{N!}\right)^{1/2} \sum_{P \in S_N} \Gamma_{\rho'\rho}^\lambda(P) P, \quad (\rho', \rho = 1, 2, \dots, f_N^\lambda), \quad (4)$$

where  $\{\Gamma_{\rho'\rho}^\lambda(P)\}$  are the matrix elements of the real orthogonal IR  $[\lambda]$  of  $S_N$ .

Let  $S$  be a specific spin state of the system in which we are interested. This corresponds to the  $IR[2^{N/2-S}1^{2S}]$  occurring in the reduction of  $v_M^r \otimes^N$ . The subset of  $v_M^r \otimes^N$  leading through Eq. (4) to a basis for such an IR cannot have an occupancy  $> 2$  for any orbital  $\phi_i$  occurring in it. Further, the number of doubly occupied orbitals, say  $p$ , has to be such that  $p \geq \frac{1}{2}N - S$ . The problem of generating these tensors is the standard one of configuration generation omitting spin projection. Any one of the standard programs can be adapted for this purpose. The characteristic feature of these tensors is that none of them are related through any permutation  $P \in S_N$ . In view of this every tensor, once generated, can be so arranged as to associate an increasing order of the electron coordinates with an increasing order of one-electron orbital indices among doubly and singly occupied parts of this

tensor. Thus a typical member of this set may be represented as

$$\Phi_{(i_p)} = \phi_{i_1}(1)\phi_{i_1}(2) \dots \phi_{i_p}(2p-1)\phi_{i_p}(2p)\phi_{i_{p+1}}(2p+1) \dots \phi_{i_{N-p}}(N) \quad (5)$$

The set of all non-zero projections

$$\{\omega_{\rho'\rho}^\lambda \Phi_{(i_p)} \mid [\lambda] = [2^{N/2-1} 2^S]; \quad \rho'\rho = 1, \dots, f_N^\lambda\}$$

can then be used to obtain the matrix elements of the Hamiltonian as [3, 12],

$$H_{\rho'\rho}^\lambda(\Phi_{(i_{p'})}; \Phi_{(i_p)}) = \left(\frac{N!}{f_N^\lambda}\right)^{1/2} \langle \Phi_{(i_{p'})} \mid H \mid \omega_{\rho'\rho}^\lambda \Phi_{(i_p)} \rangle \quad (6)$$

The Hamiltonian of Eq. (6) can, in turn, be expressed in terms of the generators of  $U_M$ ,  $\{C_{lm} \mid l, m = 1, 2, \dots, M\}$ , as [5],

$$H = \sum_{lm} f_{lm} C_{lm} + \frac{1}{2} \sum_{klmn} g_{kl;mn} (C_{ln} C_{km} - \delta_{kn} C_{lm}), \quad (7)$$

where the  $C_{lm}$  can be defined in terms of the boson operators,  $a_{i_\mu}$  acting on  $\phi_i(r_\mu)$  as [5, 7],

$$C_{lm} = \sum_{\mu=1}^N a_{i_\mu}^\dagger a_{m_\mu}. \quad (8)$$

In Eq. (7),  $f_{lm}$  and  $g_{kl;mn}$  are the standard one- and two-electron integrals.

The  $C_{lm}$  are symmetric in the electron coordinates and commute with every  $\omega_{\rho'\rho}^\lambda$ . Secondly, they act as shift operator replacing a  $\phi_m(r_k) \in \Phi_{(i_p)}$  by  $\phi_l(r_k)$  symmetrically. Since the occupancy  $N_m \geq 2$ , only  $N_m = 2, 1$  are possible if  $C_{lm} \Phi_{(i_p)} \neq 0$  for  $l \neq m$ . Thirdly, since  $\omega_{\rho'\rho}^\lambda$  does not admit a symmetrizer over more than two electron coordinates,  $N_l = 1, 0$  are only possible. Thus we need only consider four distinct cases of  $N_l, N_m$  for the effect of  $C_{lm}$  on  $\Phi_{(i_p)}$  for  $l \neq m$ . Finally,  $C_{lm}$  can at most change the pairing index  $p$  of  $\Phi_{(i_p)}$  to  $p' = p \pm 1$ . We can in this case readily show that consistency with the normalization used in Eq. (4) requires an additional renormalization factor  $\sqrt{2}$ . Based on the above considerations the effect of  $C_{lm}$  on  $\Phi_{(i_p)}$  can be determined as follows:

### 1. $N_m = 1, N_l = 0$

The effect of  $C_{lm}$  in this case is only to alter the singly occupied portion of  $\Phi_{(i_p)}$ . Hence we need number the electron coordinates of the singly occupied part alone as  $\phi_{i_{p+1}}(r_1), \phi_{i_{p+2}}(r_2), \dots, \phi_{i_{p+m}}(r_m), \dots, \phi_{i_{N-p}}(r_{N-2p})$  and introduce a compact notation. Let  $\Phi_{(i_p | m; r_m)}$  represent explicitly the fact that the reference orbital  $\phi_{p+m} \in \Phi_{(i_p)}$ . Then, using the definition and the properties of  $C_{lm}$  outlined previously, we have

$$C_{lm} \omega_{\rho'\rho}^\lambda \mid \Phi_{(i_p | m; r_m)} \rangle = \omega_{\rho'\rho}^\lambda \mid \Phi_{(i_p | l; r_m)} \rangle \quad (9)$$

In Eq. (9),  $\Phi_{(i_p | l; r_m)}$  is related through a cyclic permutation,

$$P = (r'_l r'_{l \pm 1} \dots r_{m \mp 1} r_m) \quad (10)$$

of the electron coordinates, to  $\Phi_{(i_p | l; r_l)} \in v_M^r \otimes^N$ . In Eq. (10)  $r'_l$  is the coordinate of

$\varphi_{i_p+1}$  in  $\Phi_{(i_p)}$ , and the upper sign is to be used if  $r'_l < r_m$  and the lower sign if  $r'_l > r_m$ . Combining Eqs. (4), (9) and (10) we get

$$C_{lm}\omega_{\rho'\rho}^\lambda | \Phi_{(i_p|m;r_m)} \rangle = \sum_{\rho''} \Gamma_{\rho'\rho}^\lambda(P)\omega_{\rho'\rho''}^\lambda | \Phi_{(i_p|l;r)} \rangle \quad (11)$$

## 2. $N_m = N_l = 1$

As in case 1 we again number only the electron coordinates of the singly occupied part of  $\Phi_{(i_p)}$  and indicate explicitly the presence of  $\phi_{p+m}(r_m)$  and  $\phi_{p+1}(r_l)$  in it as  $\Phi_{(i_p|l,m;r_1,r_m)}$ . Let us now introduce the permutation

$$P = (r_2 r_3 \dots \bar{r}_l)(r_1 r_2 \dots r_m), \quad (12)$$

where  $\bar{r}_l$  is the coordinate of  $\phi_{p+1}$  in  $(r_1 r_2 \dots r_m)\Phi_{(i_p|l,m;r_1,r_m)}$ . Then using the definition of  $C_{lm}$  and  $\omega_{\rho'\rho}^\lambda$  given previously we obtain

$$C_{lm}\omega_{\rho'\rho}^\lambda | \Phi_{(i_p|l,m;r_1,r_m)} \rangle = \sqrt{2} \sum_{\rho''} \Gamma_{\rho'\rho}^\lambda(P)\omega_{\rho'\rho''}^\lambda | \Phi_{(i_p|l,l;r_1,r_2)} \rangle. \quad (13)$$

In Eq. (13)  $\Phi_{(i_p|l,l;r_1,r_2)}$  does not belong to the particular class of tensors chosen since it does not have the doubly occupied orbitals  $\phi_{p+1}^2$  in the proper ordering. But there exists a simple identity valid for doubly occupied orbitals, which permits us to rearrange these orbitals without any additional effort. Let  $R_1, R_2, R_3$  and  $R_4$  be the electron coordinates of two adjacently placed doubly occupied orbitals  $\phi_{i_m}^2$  and  $\phi_{i_{m+1}}^2$  belonging to  $\Phi_{(i_p)}$ . Then using a coset decomposition of the permutation group  $S_4$  on these coordinates with respect to  $S_2 \otimes S_2$ , taken on the pairs  $R_1, R_2$  and  $R_3, R_4$ , it is easy to show that,

$$\omega_{\rho'\rho}^\lambda(R_1, R_3)(R_2, R_4) | \Phi_{(i_p)} \rangle = \omega_{\rho'\rho}^\lambda | \Phi_{(i_p)} \rangle, \quad (14)$$

where  $(R_1, R_3)$  and  $(R_2, R_4)$  are transpositions. This identity permits us to move  $\phi_{p+1}^2$  successively to the left among the doubly occupied orbitals until it reaches its proper position without affecting the right side of Eq. (13) in any way.

## 3. $N_m = 2, N_l = 0$

This case may be treated as the adjoint of 2 above in the context of evaluating the right side of Eq. (6).

## 4. $N_m = 2, N_l = 1$

Let the reference function in this case be represented as  $\Phi_{(i_p|m,m,l;R_m,R_{m+1},r_l)}$ . Using a coset decomposition of  $S_3$  on  $R_m, R_{m+1}, r_l$  with respect to the subgroup  $S_2$  on  $R_m, R_{m+1}$  and the properties of  $\omega_{\rho'\rho}^\lambda$  [3] we can readily establish the identity,

$$\omega_{\rho'\rho}^\lambda[(R_m, r_l) + (R_{m+1}, r_l)][e + (R_m, R_{m+1})] = -\omega_{\rho'\rho}^\lambda[e + (R_m, R_{m+1})]. \quad (15)$$

Since the symmetrizer  $[e + (R_m, R_{m+1})]$  occurring on the right side of Eq. (15) leaves the reference function unchanged we can replace  $C_{lm}\omega_{\rho'\rho}^\lambda | \Phi_{(i_p|m,m,l;R_m,R_{m+1},r_l)} \rangle$

by the left side of Eq. (15). This replacement, combined with the identity given in Eq. (14) enables us to show that

$$C_{lm}\omega_{\rho',\rho}^{\lambda}|\Phi_{(i_p|m,m,l;R_m,R_{m+1},r_l)}\rangle = -\sum_{\rho''}\Gamma_{\rho'',\rho}^{\lambda}(P)\omega_{\rho',\rho''}^{\lambda}|\Phi_{(i_p|l,l,m;R_l,R_{l+1},r'_m)}\rangle \quad (16)$$

where  $P$  is a cyclic permutation.

$$P=(r_l r_{l\pm 1} \dots r'_{m\mp 1} r'_m), \quad (17)$$

with a structure similar to that of Eq. (10).

Eqs. (10), (12) and (17) show that the evaluation of  $C_{lm}$  involves only permutations over singly occupied orbitals. Even though the doubly occupied coordinate indices were introduced in the case 4 we find that the final result does not involve them. In the further development the coordinates  $R_m$ ,  $R_{m+1}$  etc., will be omitted in indicating the presence of  $\phi_{i_m}^2$ , etc., in  $\Phi_{(i_p)}$ .

Since the Hamiltonian of Eq. (7) is at most quadratic in  $C_{lm}$  the above procedure can be readily extended to obtain the right side of Eq. (6). This also implies that only a limited number of basic inter-configuration matrix elements need be listed from which every matrix element can be determined. For computational convenience we found 14 basic types of  $H_{\rho',\rho}^{\lambda}(\Phi_{(i_p')}; \Phi_{(i_p)})$  to be necessary instead of the 10 suggested by Gallup and Norbeck [1]. Using the notation that the entries in the parentheses,  $(\ )$ ,  $\Phi_{(i_p)}$ ,  $\Phi_{(i_p')}$  represent the only differing orbitals and their occupancies in the two reference configurations we have listed the basic expressions in the Appendix.

As an illustration of the method of obtaining the expressions listed in the Appendix, we consider the case of Eq. (A11). Here, the initial and final states differ by two orbitals so that the part of Eq. (7) which contributes non-zero matrix elements is given by:

$$H=g_{kl;mn}C_{ln}C_{km}+g_{kl;nm}C_{lm}C_{kn}. \quad (18)$$

Using the commutation relations among the generators, we may reexpress Eq. (18) as,

$$H=(g_{kl;mn}-g_{kl;nm})C_{ln}C_{km}+g_{kl;nm}(C_{lm}C_{km}C_{mn}-C_{mn}C_{lm}C_{km}). \quad (19)$$

We now have,

$$\begin{aligned} C_{ln}C_{km}\omega_{\rho',\rho}^{\lambda}\Phi_{i_p}(m^2;kr_k;nr_n) \\ &= -C_{ln}\omega_{\rho',\rho}^{\lambda}\Phi_{i_p}(k^2;mr_k;nr_n) \\ &= -\omega_{\rho',\rho}^{\lambda}\Phi_{i_p}(k^2;mr_k;lr_n) \\ &= -\sum_{\rho''}\Gamma_{\rho'',\rho}^{\lambda}(P)\omega_{\rho',\rho''}^{\lambda}\Phi_{i_p}(k^2;mr_m;lr_l), \end{aligned} \quad (20)$$

where  $P$  is the permutation in Eq. (A11). Further,

$$C_{lm}C_{km}C_{mn}\omega_{\rho',\rho}^{\lambda}\Phi_{i_p}(m^2;kr_k;nr_n)=0, \quad (21)$$

since  $C_{mn}$  increases the orbital occupancy of  $\phi_m$  in  $\Phi_{i_p}$  to 3. Finally,

$$\begin{aligned}
 & C_{mn}C_{lm}C_{km}\omega_{\rho'\rho}^\lambda\Phi_{i_p}(m^2; kr_k; nr_n) \\
 &= -C_{mn}C_{lm}\omega_{\rho'\rho}^\lambda\Phi_{i_p}(k^2; mr_k; nr_n) \\
 &= -C_{mn}\omega_{\rho'\rho}^\lambda\Phi_{i_p}(k^2; lr_k; nr_n) \\
 &= -\omega_{\rho'\rho}^\lambda\Phi_{i_p}(k^2; lr_k; mr_n) \\
 &= -\sum_{\rho''} \Gamma_{\rho''\rho}^\lambda(PP_{(km)})\omega_{\rho'\rho''}^\lambda\Phi_{i_p}(k^2; lr_l; mr_m)
 \end{aligned} \tag{22}$$

with  $P_{(kn)}$  as the transposition  $(r_k, r_n)$  and  $P$  as defined earlier.

Using the orthogonality of the orbitals, we obtain Eq. (A11) by combining the results of Eqs. (19)–(22) in Eq. (6). The other expressions given in the Appendix have been obtained using similar methods.

### 3. Discussion

The study of CI problems in molecules is a complex one, whichever approach one uses. In the unitary group approach, the use of permutations is avoided, but one is faced with the problem of generating the lexical Gelfand-Zetlin basis [8, 9]. Further, in this approach, the matrix elements of non-elementary generators have to be handled only through the elementary ones. This could prove a difficult problem for large systems. On the other hand, the direct use of the permutation groups [3] requires that each CI matrix element be handled individually. Gallup and Norbeck [1] got over this difficulty by classifying the CI matrix elements into 10 basic categories. They did not, however, specify the explicit form of the permutations which are likely to be encountered. In this note the identities Eqs. (14) and (15) were combined with the use of the unitary group generators to obtain explicit forms for these permutations. The idea behind the use of the standard  $IR$ 's of  $S_N$  combined with the use of the model Hamiltonian is the equivalence between the Gelfand-Zetlin basis and the standard Young-Yamanouchi basis for a given configuration [7, 13].

Part of the programming for CI calculations has been done based on the present approach. All the Hamiltonian matrix elements given in the Appendix have been programmed. In obtaining these we have used the Rumer basis [14, 15] and subsequent Schmidt orthogonalization for general permutations and a recently developed method for handling general transpositions of  $S_N$  [16]. An alternative is to generate the Yamanouchi-Kotani spin functions genealogically [17] or directly [18] and use them to handle the required permutations. We are currently investigating these alternatives.

The time required to generate the Hamiltonian matrix elements compares favourably with other methods. The program and other details will be communicated in a forthcoming note.

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## Appendix

Listed below are the 14 categories of CI matrix elements. The entries in the parentheses of  $\Phi_{(i)}$  etc. list the reference orbitals and the electron coordinates. For doubly occupied orbitals the electron coordinates are not listed for the reason mentioned in the text.

$$H_{\rho'\rho}^{\lambda}(\Phi_{i_p}; \Phi_{i_p}) = \sum_i N_i \left\{ \left[ f_{ii} + (N_i - 1)J_{ii} + \sum_{\substack{j \\ (j < i)}} N_j (J_{ij} + A_{ij}K_{ij}) \right] \delta_{\rho'\rho} + \sum_{\substack{j \\ (j < i)}} N_j (2 - N_i)(2 - N_j) K_{ij} \Gamma_{\rho'\rho}^{\lambda}(P_{(ij)}) \right\} \quad (\text{A1})$$

where

$$A_{ij} = \frac{(1 - N_i)N_i + (1 - N_j)N_j}{4[2 - (N_i + N_j - 4)^2]}$$

and  $P_{(ij)}$  is the transposition of the coordinates of  $\phi_{i_{p+i}}(r_i)$ ,  $\phi_{i_{p+j}}(r_j) \in \Phi_{i_p}$ .

$$H_{\rho'\rho}^{\lambda}(\Phi_{i_{p+1}(l^2)}; \Phi_{i_p(lr_i; mr_m)}) = \sqrt{2} \left\{ f_{lm} + \sum_{\substack{i \\ (i \neq l, m)}} N_i g_{il; im} - \frac{1}{2} \sum_i N_i (N_i - 1) g_{il; mi} \right\} \Gamma_{\rho'\rho}^{\lambda}(P) + \sqrt{2} \sum_{\substack{i \\ (i \neq m)}} N_i (2 - N_i) g_{il; mi} \Gamma_{\rho'\rho}^{\lambda}(PP_{(im)}), \quad (\text{A2})$$

where  $P$  is given by Eq. (12).

$$H_{\rho'\rho}^{\lambda}(\Phi_{i_p(lr_i)}; \Phi_{i_p(mr_m)}) = \left\{ f_{lm} + \sum_{\substack{i \\ (i \neq m)}} N_i g_{il; im} - \frac{1}{2} \sum_i N_i (N_i - 1) g_{il; mi} \right\} \Gamma_{\rho'\rho}^{\lambda}(P) + \sum_{\substack{i \\ (i \neq m)}} N_i (2 - N_i) g_{il; mi} \Gamma_{\rho'\rho}^{\lambda}(PP_{(im)}), \quad (\text{A3})$$

where  $P$  is given by Eq. (10).

$$H_{\rho'\rho}^{\lambda}(\Phi_{i_p(m^2; lr_i)}; \Phi_{i_p(l^2; mr_m)}) = \left\{ -f_{ml} - \sum_{\substack{i \\ (i \neq l)}} N_i g_{im; il} - g_{lm; ll} + \frac{1}{2} \sum_{\substack{i \\ (i \neq l)}} N_i (N_i - 1) g_{im; li} \right\} \Gamma_{\rho'\rho}^{\lambda}(P) + \sum_{\substack{i \\ (i \neq m)}} N_i (N_i - 2) g_{im; li} \Gamma_{\rho'\rho}^{\lambda}(P(e + P_{(im)})), \quad (\text{A4})$$

where  $P$  is the same as that defining (A3).

$$H_{\rho',\rho}^\lambda(\Phi_{i_p(l^2)}; \Phi_{i_p(m^2)}) = g_{ll;mm} \delta_{\rho',\rho} \quad (\text{A5})$$

$$H_{\rho',\rho}^\lambda(\Phi_{i_{p+1}(k^2;l^2)}; \Phi_{i_p(m^2;kr_l;lr_l)}) = -\sqrt{2}g_{kl;mm} \Gamma_{\rho',\rho}^\lambda(P), \quad (\text{A6})$$

where

$$p = (r_2 r_3 \dots r_k)(r_1 r_2 r_3 \dots r_l)$$

is similar to Eq. (12).

$$H_{\rho',\rho}^\lambda(\Phi_{i_p(k^2;lr_l)}; \Phi_{i_p(l^2;mr_m)}) = -g_{kk;ml} \Gamma_{\rho',\rho}^\lambda(P), \quad (\text{A7})$$

with  $P$  the same as that defining (A3).

$$H_{\rho',\rho}^\lambda(\Phi_{i_{p+1}(k^2)}; \Phi_{i_p(lr_l;mr_m)}) = \sqrt{2}g_{kk;lm} \Gamma_{\rho',\rho}^\lambda(P), \quad (\text{A8})$$

where  $P$  is given by Eq. (12).

$$H_{\rho',\rho}^\lambda(\Phi_{i_p(kr_k;lr_l)}; \Phi_{i_p(mr_m;nr_n)}) = g_{kl;mn} \Gamma_{\rho',\rho}^\lambda(P) + g_{kl;nm} \Gamma_{\rho',\rho}^\lambda(PP_{(mn)}), \quad (\text{A9})$$

where

$$P = (r'_l r'_{l\pm 1} \dots \bar{r}_n)_{(r_k)} (r'_k r'_{k\pm 1} \dots r_m)$$

with  $\bar{r}_n$  as the coordinate of  $\phi_{i_{p+n}}$  in

$$(r'_k r'_{k\pm 1} \dots r_m) \Phi_{i_p(mr_m;nr_n)}$$

and

$$(r'_l r'_{l\pm 1} \dots \bar{r}_n)_{(r_k)}$$

implying the omission of  $r'_k$  from the cycle.

$$H_{\rho',\rho}^\lambda(\Phi_{i_{p+1}(k^2;lr_l)}; \Phi_{i_p(kr_k;mr_m;nr_n)}) = \sqrt{2}g_{kl;mn} \Gamma_{\rho',\rho}^\lambda(P) + \sqrt{2}g_{kl;nm} \Gamma_{\rho',\rho}^\lambda(PP_{(mn)}), \quad (\text{A10})$$

where

$$P = (\bar{r}'_l \bar{r}'_{l\pm 1} \dots \bar{r}_n) (r_2 r_3 \dots \bar{r}_k) (r_1 r_2 \dots r_m)$$

with  $\bar{r}_k$  as the coordinate of  $\phi_{i_{p+k}}$  in  $(r_1 r_2 \dots r_m) \Phi_{i_p}$ ,  $\bar{r}_n$  as the coordinate of  $\phi_{i_{p+n}}$  in  $(r_2 r_3 \dots \bar{r}_k) (r_1 r_2 \dots r_m) \Phi_{i_p}$ , and  $\bar{r}'_l = r'_l + 2$  for  $\phi_{i_{p+1}}(r'_l) \in \Phi_{i_{p+1}}$ .

$$H_{\rho',\rho}^\lambda(\Phi_{i_p(k^2;lr_l;mr_m)}; \Phi_{i_p(m^2;kr_k;nr_n)}) = -g_{kl;mn} \Gamma_{\rho',\rho}^\lambda(P) + g_{kl;nm} [\Gamma_{\rho',\rho}^\lambda(P) + \Gamma_{\rho',\rho}^\lambda(PP_{(kn)})], \quad (\text{A11})$$

where

$$P = (r'_m r'_{m\pm 1} \dots \bar{r}_k)_{(r_l)} (r'_l r'_{l\pm 1} \dots r_n). \\ H_{\rho',\rho}^\lambda(\Phi_{i_{p+2}(k^2;l^2)}; \Phi_{i_p(kr_k;lr_l;mr_m;nr_n)}) = 2g_{kl;mn} \Gamma_{\rho',\rho}^\lambda(P) + 2g_{kl;nm} \Gamma_{\rho',\rho}^\lambda(PP_{(mn)}) \quad (\text{A12})$$

where

$$P = (r_4 r_5 \dots \bar{r}_l) (r_3 r_4 \dots \bar{r}_n) (r_2 r_3 \dots \bar{r}_k) (r_1 r_2 \dots r_m),$$



with  $\bar{r}_k$  as the coordinate of  $\phi_{i_p+k}$  in  $(r_1 r_2 \dots r_m) \Phi_{i_p}$ ,  $\bar{r}_n$  as the coordinate of  $\phi_{i_p+n}$  in  $(r_2 r_3 \dots \bar{r}_k)(r_1 r_2 \dots r_m) \Phi_{i_p}$ , and  $\bar{r}$  as the coordinate of  $\phi_{i_p+i}$  in

$$(r_3 r_4 \dots \bar{r}_n)(r_2 r_3 \dots \bar{r}_k)(r_1 r_2 \dots r_m) \Phi_{i_p} \cdot \\ H_{\rho'\rho}^\lambda(\Phi_{i_p+1}(k^2; l^2; mr'_m); \Phi_{i_p}(m^2; kr_k; lr_l; nr_n)) \\ = -\sqrt{2}g_{kl; mn} \Gamma_{\rho'\rho}^\lambda(P) - \sqrt{2}g_{kl; nm} \Gamma_{\rho'\rho}^\lambda(PP_{(kl)}), \quad (A13)$$

where

$$P = (\tilde{r}'_m \tilde{r}'_{m\pm 1} \dots \bar{r}_k)(r_2 r_3 \dots \bar{r}_l)(r_1 r_2 \dots r_n) \cdot \\ H_{\rho'\rho}^\lambda(\Phi_{i_p}(k^2; l^2; mr'_m; nr'_n); \Phi_{i_p}(m^2; n^2; kr_k; lr_l)) \\ = g_{kl; mn} \Gamma_{\rho'\rho}^\lambda(P) + g_{lk; mn} \Gamma_{\rho'\rho}^\lambda(PP_{(kl)}), \quad (A14)$$

where

$$P = (r'_m r'_{m\pm 1} \dots \bar{r}_k)_{(r'_n)} (r'_n r'_{n\pm 1} \dots r_1).$$

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