BASIC EXCHANGE INTEGRALS AND THE TRIPLE DOUBLE COSET SYMBOL

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Definition: TRIPLE DOUBLE COSET SYMBOL.

Any set of semidefinite positive integers D_{jkl} $1 \leqslant j,k,l \leqslant s,t,v$ is called a TDCS if the sets D_{jko}, D_{jol} and D_{okl} obtained by summing D_{jkl} over l, k and j respectively, are ordinary DCS with respect to the sets D_{joo}, D_{oko} and D_{ool} which are partitions of $D_{ooo} = N$. The sets D_{jko}, D_{jol} and D_{okl} will be called the projections of the TDCS.

Let $D_{joo} \Rightarrow H^{\alpha}$, $D_{oko} \Rightarrow H^{\beta}$ and $D_{ool} \Rightarrow H^{\gamma}$ define subgroups of $G = S_N$, which are direct products of symmetric groups of degree D_{joo} $j = 1,2,\ldots s$, D_{oko} $k = 1,2,\ldots t$ and D_{ool} $l = 1,2,\ldots v$, respectively.

THEOREM. (1)

$H^{\alpha} W_c^{\alpha\beta} H^{\beta} \Leftrightarrow D(W_c^{\alpha\beta})$; elements $D_{jko}(W_c^{\alpha\beta})$; $D^t(W_c^{\alpha\beta}) = D(W_{\bar{c}}^{\beta\alpha}) \Leftrightarrow H^{\beta} W_{\bar{c}}^{\beta\alpha} H^{\alpha}$, which expresses the fact that DC and DCS correspond uniquely [1]. Similar correspondences are obtained by cyclically permuting α, β and γ.

Let the TDCS for two *fixed* projections, say $W_a^{\beta\gamma}$ and $W_b^{\gamma\alpha}$ be denoted by $D(W_a^{\beta\gamma}, W_b^{\gamma\alpha}; Z)$.

THEOREM. (2)

The TDCS $D(W_a^{\beta\gamma}, W_b^{\gamma\alpha}; Z)$ are 1-to-1 corresponding to the DC $H_b^{\gamma\alpha} Z H_{\bar{a}}^{\gamma\beta}$ (or their inverses) in the decomposition of H^{γ} with respect to $H_b^{\gamma\alpha} = H^{\gamma} \cap W_b^{\gamma\alpha} H^{\alpha} W_{\bar{b}}^{\alpha\gamma}$ on the left and $H_{\bar{a}}^{\gamma\beta} = H^{\gamma} \cap W_{\bar{a}}^{\gamma\beta} H^{\beta} W_a^{\beta\gamma}$ on the right, i.e.,

$$D(W_a^{\beta\gamma}, W_b^{\gamma\alpha}; Z) \Leftrightarrow H_b^{\gamma\alpha} Z H_{\bar{a}}^{\gamma\beta} .$$

Similar correspondences are obtained by cyclically permuting α, β and γ.

Definition: BASIC EXCHANGE INTEGRAL.

Let $\phi^{\alpha} = \ldots \bullet \; \phi_i^{\alpha} \ldots \phi_j^{\alpha} \bullet \ldots$ denote an N-particle orbital product in which orbital ϕ_j^{α} occurs D_{joo} times, i.e., ϕ_j^{α} is occupied by D_{joo} particles. Then H^{α} is the invariance group of ϕ^{α}, which means $g\phi^{\alpha} = \phi^{\alpha} \; \forall g \in H^{\alpha}$. We use the notation $\phi^{\alpha} = |\phi^{\alpha}; \lambda_t^{\alpha})$, where the symmetry of ϕ^{α} is denoted by λ_t^{α}, the trivial irreducible representation (IR) of the invariance group H^{α}.

Let $|\phi^{\alpha}(k^{\alpha}\lambda_t^{\alpha}); \Lambda J) = Q(J\Lambda k^{\alpha}\lambda_t^{\alpha}) |\phi^{\alpha}; \lambda_t^{\alpha})$ denote the k^{α}-th linearly indepent N-particle function of final symmetry ΛJ of G $(= S_N)$, obtained by projection with $Q(J\Lambda k^{\alpha}\lambda_t^{\alpha})$, a sequence-$(H^{\alpha} \subset G)$-adapted matric basis element [2], from the product $|\phi^{\alpha}; \lambda_t^{\alpha})$. The range of k^{α} is given by $\langle \Lambda | \lambda_t^{\alpha} \uparrow \rangle$, the frequency of induction. Similarly ϕ^{β}, etc., is defined.

Let Ω_{γ} denote the totally symmetric spin-free γ-particle operator and ω_{γ} the corresponding prototype operator defined with respect to γ fixed particle labels. The invariance group of ω_{γ} is denoted by H^{γ} $(= S_{\gamma} \times S_{N-\gamma})$. Then, in the "separation of the last γ particles" scheme [3], one obtains the following non-vanishing matrix elements:

$$|G|(|H^\alpha||H^\beta||H^\gamma|)^{-1}(\phi^\alpha(k^\alpha\lambda_t^\alpha);\Lambda\,||\,\Omega_\gamma\,||\,\phi^\beta(k^\beta\lambda_t^\beta);\Lambda) =$$

$$= \sum_{\bar a}\sum_{\bar b}\Big\{\sum_{\bar z}\bar f_{\bar z}\langle W_{\bar b}^{\alpha\gamma} Z\, W_{\bar a}^{\gamma\beta}\,|\,k^\alpha\lambda_t^\alpha\Lambda\, k^\beta\lambda_t^\beta\rangle\,(\phi^\alpha;\lambda_t^\alpha\,|\,W_{\bar b}^{\alpha\gamma} Z\,\omega_\gamma\, W_{\bar a}^{\gamma\beta}\,|\,\phi^\beta;\lambda_t^\beta)\Big\} \tag{3}$$

where

$W_{\bar b}^{\alpha\gamma}$ ranges over the DC in the decomposition $G \bmod (H^\alpha,H^\gamma)$

$W_{\bar a}^{\gamma\beta}$ ranges over the DC in the decomposition $G \bmod (H^\gamma,H^\beta)$, and, for *fixed* $W_{\bar b}^{\alpha\gamma}$ and $W_{\bar a}^{\gamma\beta}$, Z ranges over the DC $H^\gamma \bmod (H_{\bar b}^{\gamma\alpha},H_{\bar a}^{\gamma\beta})$.

The integrals $(\phi^\alpha;\lambda_t^\alpha\,|\,W_{\bar b}^{\alpha\gamma} Z\,\omega_\gamma\, W_{\bar a}^{\gamma\beta}\,|\,\phi^\beta;\lambda_t^\beta)$ are the BEI. These cannot be simplified further without additional information concerning the orbitals ϕ_j^α in ϕ^α and ϕ_k^β in ϕ^β. The expansion coefficients are matrix elements of triple products of DC generators in the IR Λ which is sequence adapted on the left and the right with respect to H^α and H^β, respectively. The numerical factor $\bar f_{\bar z}$ is treated in the following

THEOREM. BEI $\Leftrightarrow$ TDCS (4)

$$f_{\bar z} = \prod_{jkl}^{s\epsilon v}\big(D_{jkl}(W_a^{\beta\gamma},W_b^{\gamma\alpha};Z)\big)!$$

The transformation from BEI to primitive integrals PI is given by the following results.

Consider the $\gamma = 0$ BEI:

With $D_{jk0}(W_c^{\alpha\beta}) = d_{jk}^c$ for short and $S_{jk} = (\phi_j^\alpha\,|\,\phi_k^\beta)$ the 1-particle overlaps, we have

$$(\phi^\alpha;\lambda_t^\alpha\,|\,W_c^{\alpha\beta}\,|\,\phi^\beta;\lambda_t^\beta) = \prod_{jk}^{s\epsilon} S_{jk}^{d_{jk}^c} \equiv S(W_c^{\alpha\beta}) \tag{5}$$

Consider the $\gamma \neq 0$ BEI:

With $Z \in H^\gamma = S_\gamma \times S_{N-\gamma}$, Z is factorized, say $Z = Y''Y'$, $Y'' \in S_\gamma$, $Y' \in S_{N-\gamma}$.

With $d'_{jk} = D_{jk1}(W_a^{\beta\gamma},W_b^{\gamma\alpha};Y'Y'')$, $d''_{jk} = D_{jk2}(W_a^{\beta\gamma},W_b^{\gamma\alpha};Y'Y'')$ for short, and the 1-particle charge contributions $\rho_{jk} = \phi_j^\alpha\phi_k^\beta$,

we have

$$(\phi^\alpha;\lambda_t^\alpha\,|\,W_{\bar b}^{\alpha\gamma}Y'\omega_\gamma Y'' W_{\bar a}^{\gamma\beta}\,|\,\phi^\beta;\lambda_t^\beta) = \Big(\prod_{jk}^{s\epsilon}\rho_{jk}^{d''_{jk}}\,\Big|\,\omega_\gamma\Big)\prod_{jk} S_{jk}^{d'_{jk}} \tag{6}$$

and since for given a and b, $Z = Y'Y''$ fixes the third projection c this can be written as

$$\frac{S(W_c^{\alpha\beta})\,J^\gamma(Y'')}{S^\gamma(Y'')} \quad \text{where} \quad S^\gamma(Y'') = \prod_{jk} S_{jk}^{d''_{jk}} \tag{7}$$

and $J^\gamma(Y'') = \Big(\prod_{jk}\rho_{jk}^{d''_{jk}}\,\Big|\,\omega_\gamma\Big)$, the PI.

After some algebra, expansion (3) can be rewritten as

$$|G|(|H^\alpha||\Lambda||H^\beta|)^{-1}(\phi^\alpha(k^\alpha\lambda_t^\alpha);\Lambda\,||\,\Omega_\gamma\,||\,\phi^\beta(k^\beta\lambda_t^\beta);\Lambda) = \tag{8}$$

$$= \sum_{c} \langle w_c^{\alpha\beta} | k^\alpha \lambda_t^\alpha \wedge k^\beta \lambda_t^\beta \rangle \, S(w_c^{\alpha\beta}) \sum_{y''} \frac{J^\gamma(y'')}{S^\gamma(y'')} \left[\prod_{jk}^{st} \frac{1}{d_{jk}^c!} \binom{d_{jk}^c}{d_{jk}''} \right]$$

which expresses the original matrix element in terms of PI. We note that only one DC decomposition occurs namely $G\,\mathrm{mod}\,(H^\alpha, H^\beta)$.

COROLLARIES AND REMARKS: [4]

1. The number of DC $G\,\mathrm{mod}\,(H^\alpha, H^\beta)$ is given by $N_G^{\alpha\beta} = \langle \lambda_t^\alpha \uparrow^G \downarrow_\beta | \lambda_t^\beta \rangle$.

   The number of TDCS = number of BEI is $N_G^{\alpha\beta\gamma} = \langle \lambda_t^\beta \uparrow^G \downarrow_\alpha \uparrow^G \downarrow_\gamma | \lambda_t^\gamma \rangle$.
2. For two fixed projections say a and b, the TDCS $D(W_a^{\beta\gamma}, W_b^{\gamma\alpha}; Z)$, Z ranging, can also be denoted by $D(W_a^{\beta\gamma}, W_b^{\gamma\alpha}, W_c^{\alpha\beta}; W)$, c and W ranging, where W distinguishes different TDCS for three fixed projections.

The quantity

$$\langle w_a^{\beta\gamma}, w_b^{\gamma\alpha}, w_c^{\alpha\beta} \rangle \equiv \sum_{W} \left\{ \prod_{jk\ell} D_{jk\ell}(w_a^{\beta\gamma}, w_b^{\gamma\alpha}, w_c^{\alpha\beta}; W)! \right\}^{-1} \tag{9}$$

is in essence a DC multiplication constant, i.e., this quantity is proportional to the coefficient with which the identity occurs in the product $H^\beta W_a^{\beta\gamma} H^\gamma \,.\, H^\gamma W_b^{\gamma\alpha} H^\alpha \,.\, H^\alpha W_c^{\alpha\beta} H^\beta$. Actually

$$|G|\,|H_a^{\beta\gamma}|\,|H_b^{\gamma\alpha}|\,|H_c^{\alpha\beta}|\,(|H^\alpha|\,|H^\beta|\,|H^\gamma|)^{-1} \langle w_a^{\beta\gamma}, w_b^{\gamma\alpha}, w_c^{\alpha\beta} \rangle = \tag{10}$$

$$= \sum_{\Lambda} |\Lambda| \sum_{k^\alpha} \sum_{k^\beta} \sum_{k^\gamma} \langle w_a^{\beta\gamma} | k^\beta \lambda_t^\beta \wedge k^\gamma \lambda_t^\gamma \rangle \langle w_b^{\gamma\alpha} | k^\gamma \lambda_t^\gamma \wedge k^\alpha \lambda_t^\alpha \rangle \langle w_c^{\alpha\beta} | k^\alpha \lambda_t^\alpha \wedge k^\beta \lambda_t^\beta \rangle,$$

in which Λ ranges over all IR of G and k^α, k^β and k^γ over the frequences of induction. The matrix elements that occur in this expansion (the basic DC constants [5]) are the same as those in expansions (3) and (8).

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