Fock space algebraic methods: Normal ordering with respect to vac and Φ

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1 Fock space

Definition 1.1. ***Fock space.*** Let $\mathcal{H}$ be a complete one-particle Hilbert space, so that $\mathcal{H}^{\otimes n} = \mathcal{H} \underset{n \text{ times}}{\otimes \cdots \otimes} \mathcal{H}$ is an n-particle Hilbert space. The space of candidate n-fermion wavefunctions in $\mathcal{H}^{\otimes n}$ is then $\mathbb{A}(\mathcal{H}^{\otimes n})$, its antisymmetric subspace. If $\{\psi_p\}$ is a complete, orthonormal basis for $\mathcal{H}$, then

$$\Phi_{(p_1 \cdots p_n)} = \frac{1}{\sqrt{n!}} \sum_{\pi}^{\mathrm{S}_n} \varepsilon_\pi \psi_{p_{\pi(1)}} \otimes \cdots \otimes \psi_{p_{\pi(n)}} \qquad \text{where } p_1 < \cdots < p_n \tag{1.1}$$

is a complete, orthonormal basis for $\mathbb{A}(\mathcal{H}^{\otimes n})$. Represented as functions of space and spin coordinates, these basis vectors become Slater determinants. The *fermionic Fock space* $F(\mathcal{H})$ over $\mathcal{H}$ is given by a direct sum of $\mathbb{A}(\mathcal{H}^{\otimes n})$ from $n = 0$ to $n = \infty$, i.e. $F(\mathcal{H}) = \mathbb{C} \oplus \mathbb{A}(\mathcal{H}^{\otimes 1}) \oplus \mathbb{A}(\mathcal{H}^{\otimes 2}) \oplus \mathbb{A}(\mathcal{H}^{\otimes 3}) \oplus \cdots$, which spans all possible fermionic wavefunctions.

Definition 1.2. ***The occupation number representation of $F(\mathcal{H})$.*** In the *occupation number representation* of Fock space, the basis vectors (equation 1.1) are represented as lists of 1s and 0s

$$|(p_1 \cdots p_n)\rangle \equiv |n_1, n_2, n_3, \ldots, n_\infty\rangle \qquad \text{where } p_1 < \cdots < p_n \text{ and } n_p = \begin{cases} 1 & \text{if } p \in (p_1 \cdots p_n) \\ 0 & \text{if } p \notin (p_1 \cdots p_n) \end{cases} \tag{1.2}$$

where $n_p = 1$ when ψ_p is occupied and $n_p = 0$ when ψ_p is unoccupied. The basis for $\mathbb{A}(\mathcal{H}^{\otimes n})$ is given by distributing n 1s in the occupation vector in all possible ways. The state in which no spin-orbitals are occupied is called the *vacuum state*, here denoted $|\mathrm{vac}\rangle$, which spans $\mathcal{H}^{\otimes 0}$ ($= \mathbb{A}(\mathcal{H}^{\otimes 0}) = \mathbb{C}$, up to isomorphism).

2 Particle-hole operators

Definition 2.1. ***Particle-hole operators.*** *Particle-hole operators* include *annihilation operators* and *creation operators*. The *annihilation operator* of ψ_p is a linear mapping $a_p : \mathbb{A}(\mathcal{H}^{\otimes n}) \to \mathbb{A}(\mathcal{H}^{\otimes (n-1)})$ defined by

$$a_p|\cdots n_p \cdots\rangle = (-)^{n_1 + \cdots + n_{p-1}}|\cdots n_p - 1 \cdots\rangle \quad \text{if } n_p = 1 \qquad a_p|\cdots n_p \cdots\rangle = 0 \quad \text{if } n_p = 0 \tag{2.1}$$

and the *creation operator* of ψ_p is a linear mapping $c_p : \mathbb{A}(\mathcal{H}^{\otimes n}) \to \mathbb{A}(\mathcal{H}^{\otimes (n+1)})$ defined by

$$c_p|\cdots n_p \cdots\rangle = (-)^{n_1 + \cdots + n_{p-1}}|\cdots n_p + 1 \cdots\rangle \quad \text{if } n_p = 0 \qquad c_p|\cdots n_p \cdots\rangle = 0 \quad \text{if } n_p = 1. \tag{2.2}$$

Proposition 2.1. $\boldsymbol{c_p = a_p^\dagger}$**.** *Creation and annihilation operators of a one-particle state ψ_p are adjoints of each other.*

Proof: $\langle n_1' n_2' \cdots | a_p [n_1 n_2 \cdots]\rangle$ vanishes unless $n_p' = 0$, $n_p = 1$, and $n_q' = n_q$ for $q \neq p$, in which case it equals $(-)^{n_1 + \cdots + n_{p-1}}$. The same is true for $\langle c_p [n_1' n_2' \cdots] | n_1 n_2 \cdots\rangle$. Therefore, $\langle \Psi | a_p \Psi'\rangle = \langle c_p \Psi | \Psi'\rangle$ for arbitrary linear combinations Ψ and Ψ' of the basis states, which implies $c_p = a_p^\dagger$ by the definition of adjoint.

Proposition 2.2. $\boldsymbol{[q, q']_+ = \delta_{q' q^\dagger}}$**.** *Particle-hole operators q and q' anticommute unless $q' = q^\dagger$, for which $[q, q^\dagger]_+ = 1$.*

Proof: Let q and q' be arbitrary particle-hole operators acting on states ψ_p and $\psi_{p'}$. First, suppose $p \neq p'$. Then

$$qq'|\cdots n_p \cdots n_{p'} \cdots\rangle = (-)^{n_p + \sum_{r=p+1}^{p'} n_r}|\cdots \overline{n_p} \cdots \overline{n_{p'}} \cdots\rangle$$
$$\text{and} \quad q'q|\cdots n_p \cdots n_{p'} \cdots\rangle = (-)^{\overline{n_p} + \sum_{r=p+1}^{p'} n_r}|\cdots \overline{n_p} \cdots \overline{n_{p'}} \cdots\rangle$$

where $\overline{n_p}$ and $\overline{n_{p'}}$ are the occupations after operating q and q' on the state. Since n_p and $\overline{n_p}$ differ by one, $qq' = -q'q$. Now, consider the case $p = p'$ which implies $q' \in \{q, q^\dagger\}$. If $q' = q$ then $qq' = -q'q = 0$. In the final case, $q' = q^\dagger$, we have either $a_p^\dagger a_p|\cdots n_p \cdots\rangle = |\cdots n_p \cdots\rangle$ and $a_p a_p^\dagger|\cdots n_p \cdots\rangle = 0$ if $n_p = 1$ or vice versa if $n_p = 0$, so that $(qq^\dagger + q^\dagger q) = 1$.

Remark 2.1. ***Representing Slater determinants in terms of particle-hole operators.*** The Slater determinant $\Phi_{(p_1 \cdots p_n)}$ can be represented in $F(\mathcal{H})$ as

$$|\Phi_{(p_1 \cdots p_n)}\rangle = a_{p_1}^\dagger \cdots a_{p_n}^\dagger |\mathrm{vac}\rangle \tag{2.3}$$

which is equivalent to $|(p_1 \cdots p_n)\rangle$ for $p_1 < \cdots < p_n$, and is otherwise equivalent to $\varepsilon_\pi |(p_{\pi(1)} \cdots p_{\pi(n)})\rangle$ for $\pi \in \mathrm{S}_n$ such that $p_{\pi(1)} < \cdots < p_{\pi(n)}$. The actions of a_p and $a_p^\dagger$ on $\Phi_{(p_1 \cdots p_n)}$ are given by

$$a_p \Phi_{(p_1 \cdots p_n)} = (-)^{k-1} \Phi_{(p_1 \cdots \cancel{p_k} \cdots p_n)} \ \text{ if } p = p_k \in (p_1 \cdots p_n) \qquad a_p \Phi_{(p_1 \cdots p_n)} = 0 \ \text{ if } p \notin (p_1 \cdots p_n) \tag{2.4}$$
$$a_p^\dagger \Phi_{(p_1 \cdots p_n)} = (-)^{k-1} \Phi_{(p_1 \cdots p_{k-1} p p_k \cdots p_n)} \ \text{ if } p \notin (p_1 \cdots p_n) \qquad a_p^\dagger \Phi_{(p_1 \cdots p_n)} = 0 \ \text{ if } p \in (p_1 \cdots p_n) \tag{2.5}$$

which follows from equation 2.3 and Prop 2.2.

Definition 2.2. vac-*normal order.* A string $q_1 \cdots q_n$ of particle-hole operators $q_i \in \{a_p\} \cup \{a_p^\dagger\}$ is in *vacuum normal order* (or vac-*normal order*) when all of its creation operators lie to the left of all of its annihilation operators. That is, a string of particle-hole operators is in vac-normal order if it has the form $a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{r_1} \cdots a_{r_{m'}}$. This guarantees that $\langle \mathrm{vac}|q_1 \cdots q_n|\mathrm{vac}\rangle = 0$, i.e. its vacuum expectation value vanishes.

Definition 2.3. *Particle-number conserving strings.* A string $q_1 \cdots q_n$ is *particle-number conserving* if it contains the same number of creation and annihilation operators, and so maps each m-particle subspace $\mathbb{A}(\mathcal{H}^{\otimes m})$ into itself.

Definition 2.4. *Excitation operators.* Excitation operators are particle-number conserving strings in normal order, i.e. strings which have have the form $a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1}$ ($= a_{p_1}^\dagger a_{q_1} \cdots a_{p_m}^\dagger a_{q_m}$ if $\{p_i\} \cap \{q_i\} = \emptyset$). For a given reference determinant Φ, excited determinants are given by $\Phi_{i_1 \cdots i_m}^{a_1 \cdots a_m} = a_{a_1}^\dagger \cdots a_{a_m}^\dagger a_{i_m} \cdots a_{i_1} \Phi$ where $i_1 \cdots i_m$ are occupied and $a_1 \cdots a_m$ are virtual indices with respect to Φ.

Remark 2.2. *The Fock space Hamiltonian.* The electronic Hamiltonian can be expressed in $F(\mathcal{H})$ as

$$H_e = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} \langle pq|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

where $h_{pq} = \langle \psi_p(1)|\hat{h}(1)|\psi_q(1)\rangle$ and $\langle pq|rs\rangle = \langle \psi_p(1)\psi_q(2)|\hat{g}(1,2)|\psi_r(1)\psi_s(2)\rangle$ are the one- and two-electron integrals.

Definition 2.5. *One-particle and one-hole density matrices.* The *one-particle* and *one-hole density matrices* of a state $\Psi \in F(\mathcal{H})$ are given by $\gamma_{pq} \equiv \langle \Psi|a_q^\dagger a_p|\Psi\rangle$ and $\eta_{pq} \equiv \langle \Psi|a_p a_q^\dagger|\Psi\rangle$, respectively.

3 vac-normal ordering

Definition 3.1. vac-*normal ordering.* The vac-*normal ordering* of a string $q_1 \cdots q_n$ of particle-hole operators is the mapping $q_1 \cdots q_n \mapsto {:}q_1 \cdots q_n{:} \equiv \varepsilon_\pi q_{\pi(1)} \cdots q_{\pi(n)}$ where $\pi \in \mathrm{S}_n$ is a permutation that places the string in normal order.

Definition 3.2. vac-*normal contraction.* A pairwise vac-*normal contraction*, $\overbracket{q_1 q_2}$, of two particle-hole operators q_1 and q_2 is defined as $\overbracket{q_1 q_2} \equiv q_1 q_2 - {:}q_1 q_2{:}$. This associates a scalar value with every pair in $\{a_p\} \cup \{a_p^\dagger\}$, of which the only non-trivial case is $\overbracket{a_p a_q^\dagger} = a_p a_q^\dagger - {:}a_p a_q^\dagger{:} = a_p a_q^\dagger + a_q^\dagger a_p = \delta_{pq}$. All other vac-normal contractions, including $\overbracket{a_p^\dagger a_q}$, are zero.

Remark 3.1. *Non-vanishing* vac-*normal contractions are elements of the* vac *one-hole density matrix.* Note that vac-normal contractions can in general be identified with $\overbracket{q_1 q_2} = \langle \mathrm{vac}|q_1 q_2 - {:}q_1 q_2{:}|\mathrm{vac}\rangle = \langle \mathrm{vac}|q_1 q_2|\mathrm{vac}\rangle$, since $\langle \mathrm{vac}|{:}q_1 q_2{:}|\mathrm{vac}\rangle = 0$ and $\overbracket{q_1 q_2}$ is a scalar. The only non-trivial contractions are those with an annihilation operator on the left and a creation operator on the right, which are elements of the one-hole density matrix $\overbracket{a_p a_q^\dagger} = \langle \mathrm{vac}|a_p a_q^\dagger|\mathrm{vac}\rangle = \eta_{pq} = \delta_{pq}$ of the vacuum.

Definition 3.3. vac-*normal ordering with contractions.* If $q_1 \cdots q_n$ is a string of particle-hole operators, its vac-*normal ordering with contraction* $\overbracket{q_i q_j}$ $(i < j)$ is defined as ${:}q_1 \cdots \overbracket{q_i \cdots q_j} \cdots q_n{:} \equiv (-)^{j-i-1} \overbracket{q_i q_j} {:}q_1 \cdots \cancel{q_k} \cdots \cancel{q_l} \cdots q_n{:}$ where the phase factor corresponds to the signature of the permutation required to bring q_i and q_j together. vac-normal-ordered products with multiple contractions are defined analogously.

Notation 3.1. Given a string $Q = q_1 \cdots q_n$ of particle-hole operators, let ${:}Q(\overbracket{q_i q_j}){:}$ denote ${:}q_1 \cdots \overbracket{q_i \cdots q_j} \cdots q_n{:}$. This is unambiguous for $i < j$. Let ${:}\overline{Q}{:}$ denote the sum of all unique single, double, triple, etc. contractions, i.e.

$${:}\overline{Q}{:} \equiv \sum_{k=1}^{\lfloor n/2 \rfloor} \sum_{\substack{i_1 \cdots i_k \\ j_1 \cdots j_k}}^{\mathrm{Ctr}_k(Q)} {:}Q(\overbracket{q_{i_1} q_{j_1}} \cdots \overbracket{q_{i_k} q_{j_k}}){:}$$

where $\mathrm{Ctr}_k(Q)$ runs over the unique sets of k pairs of operator indices in Q and $\lfloor\rfloor$ is the floor function. Let ${:}\overline{\overline{Q}}{:}$ denote the sum of all *complete contractions* of Q, i.e. the terms in ${:}\overline{Q}{:}$ in which all operators in the product are involved in a contraction. For a pair of particle-hole operator strings Q and Q', let ${:}\overbracket{QQ'}{:}$ denote the sum of all *cross contractions* between Q and Q' in ${:}\overline{QQ'}{:}$, i.e. omitting any *internal contractions* in Q or Q'. Finally, let ${:}\overline{\overbracket{QQ'}}{:}$ denote the sum of *complete cross contractions* between Q and Q' in ${:}\overbracket{QQ'}{:}$, i.e. those in which every operator in Q is contracted with an operator in Q' and no uncontracted operators are left over.

4 Wick's theorem

Lemma 4.1. $\mathbf{:}Q\mathbf{:}q = \mathbf{:}Qq\mathbf{:} + \sum_k \mathbf{:}Q(\overbrace{q_k)q}\mathbf{:}$

Proof: We can assume without loss of generality that Q is already in normal order so that $\mathbf{:}Q\mathbf{:} = Q$. Let n be the number of operators in Q. If q is an annihilation operator then $\mathbf{:}Qq\mathbf{:} = Qq$ and all of the contractions between Q an q vanish (see Def 3.2), so the statement is trivially true. If q is a creation operator then $\mathbf{:}Qq\mathbf{:} = (-)^n qQ$, and

$$Qq = (-)^n qQ + \sum_{k=1}^{n} (-)^{n-k} q_1 \cdots [q_k, q]_+ \cdots q_n = \mathbf{:}Qq\mathbf{:} + \sum_{k=1}^{n} \mathbf{:}Q(\overbrace{q_k)q}\mathbf{:}$$

using the pull-through relation (see Prop A.1), the fact that $\mathbf{:}Q(\overbrace{q_k)q}\mathbf{:} = (-)^{n-k} q_1 \cdots \overbrace{q_k q} \cdots q_n$, and the fact that $\overbrace{q_k q} = [q_k, q]_+$ when q is a creation operator (see again Def 3.2).

Theorem 4.1. ***Wick's Theorem, $Q = \mathbf{:}Q\mathbf{:} + \mathbf{:}\overline{Q}\mathbf{:}$ (time-independent).*** *Any string Q of particle-hole operators is equal to $\mathbf{:}Q\mathbf{:} + \mathbf{:}\overline{Q}\mathbf{:}$, its normal-ordered form plus the sum of all possible contractions.*

Proof: Let $Q = q_1 \cdots q_n$. The result holds for $n = 2$ because $q_1 q_2 = \mathbf{:}q_1 q_2\mathbf{:} + \overbrace{q_1 q_2}$ follows immediately from Def 3.2. Now, assume it holds for Q with n operators and consider Qq. By our inductive assumption $Qq = \mathbf{:}Q\mathbf{:}q + \mathbf{:}\overline{Q}\mathbf{:}q$. Applying Lem 4.1 to $\mathbf{:}Q\mathbf{:}q$, we find $\mathbf{:}Q\mathbf{:}q = \mathbf{:}Qq\mathbf{:} + \sum_i \mathbf{:}Q(\overbrace{q_i)q}\mathbf{:}$. Expanding $\mathbf{:}\overline{Q}\mathbf{:}q$ and applying Lem 4.1 to each term gives

$$\sum_{k=1}^{\lfloor n/2 \rfloor} \sum_{\substack{i_1 \cdots i_k \\ j_1 \cdots j_k}}^{\mathrm{Ctr}_k(Q)} \mathbf{:}Q(\overbrace{q_{i_1} q_{j_1}} \cdots \overbrace{q_{i_k} q_{j_k}})\mathbf{:}q = \sum_{k=1}^{\lfloor n/2 \rfloor} \sum_{\substack{i_1 \cdots i_k \\ j_1 \cdots j_k}}^{\mathrm{Ctr}_k(Q)} \mathbf{:}Q(\overbrace{q_{i_1} q_{j_1}} \cdots \overbrace{q_{i_k} q_{j_k}})q\mathbf{:} + \sum_{k=1}^{\lfloor n/2 \rfloor} \sum_{\substack{i_1 \cdots i_k \\ j_1 \cdots j_k}}^{\mathrm{Ctr}_k(Q)} \sum_{i \notin \{ \substack{i_1 \cdots i_k \\ j_1 \cdots j_k} \}} \mathbf{:}Q(\overbrace{q_{i_1} q_{j_1}} \cdots \overbrace{q_{i_k} q_{j_k}} \overbrace{q_i)q}\mathbf{:}$$

$$= \sum_{\substack{i_1 \\ j_1}}^{\mathrm{Ctr}_1(Q)} \mathbf{:}Q(\overbrace{q_{i_1} q_{j_1}})q\mathbf{:} + \sum_{k=2}^{\lfloor (n+1)/2 \rfloor} \sum_{\substack{i_1 \cdots i_k \\ j_1 \cdots j_k}}^{\mathrm{Ctr}_k(Qq)} \mathbf{:}Qq(\overbrace{q_{i_1} q_{j_1}} \cdots \overbrace{q_{i_k} q_{j_k}})\mathbf{:}$$

and, combining these results, we find

$$Qq = \mathbf{:}Q\mathbf{:}q + \mathbf{:}\overline{Q}\mathbf{:}q = \mathbf{:}Qq\mathbf{:} + \sum_i \mathbf{:}Q(\overbrace{q_i)q}\mathbf{:} + \sum_{\substack{i_1 \\ j_1}}^{\mathrm{Ctr}_1(Q)} \mathbf{:}Q(\overbrace{q_{i_1} q_{j_1}})q\mathbf{:} + \sum_{k=2}^{\lfloor (n+1)/2 \rfloor} \sum_{\substack{i_1 \cdots i_k \\ j_1 \cdots j_k}}^{\mathrm{Ctr}_k(Qq)} \mathbf{:}Qq(\overbrace{q_{i_1} q_{j_1}} \cdots \overbrace{q_{i_k} q_{j_k}})\mathbf{:}$$

$$= \mathbf{:}Qq\mathbf{:} + \sum_{k=1}^{\lfloor (n+1)/2 \rfloor} \sum_{\substack{i_1 \cdots i_k \\ j_1 \cdots j_k}}^{\mathrm{Ctr}_k(Qq)} \mathbf{:}Qq(\overbrace{q_{i_1} q_{j_1}} \cdots \overbrace{q_{i_k} q_{j_k}})\mathbf{:}$$

which is $\mathbf{:}Qq\mathbf{:} + \mathbf{:}\overline{Qq}\mathbf{:}$. So if the statement holds for strings of length n it must also hold for strings of length $n+1$ and, by induction, the theorem holds for Q of arbitary length.

Corollary 4.1. ***Wick's Theorem for operator products.*** *Given a pair Q, Q' of particle-hole operator strings already in normal order, the product of their normal orderings is given by $\mathbf{:}Q\mathbf{::}Q'\mathbf{:} = \mathbf{:}QQ'\mathbf{:} + \mathbf{:}\overbrace{Q}\overbrace{Q'}\mathbf{:}$.*

Proof: By Wick's theorem $\mathbf{:}Q\mathbf{::}Q'\mathbf{:} = \mathbf{:}QQ'\mathbf{:} + \mathbf{:}\overline{(\mathbf{:}Q\mathbf{::}Q'\mathbf{:})}\mathbf{:}$. Since $\mathbf{:}Q\mathbf{:}$ and $\mathbf{:}Q'\mathbf{:}$ are in normal order their internal contractions in $\mathbf{:}\overline{(\mathbf{:}Q\mathbf{::}Q'\mathbf{:})}\mathbf{:}$ vanish, which implies $\mathbf{:}\overline{(\mathbf{:}Q\mathbf{::}Q'\mathbf{:})}\mathbf{:} = \mathbf{:}\overbrace{Q}\overbrace{Q'}\mathbf{:}$.

Corollary 4.2. $\langle \mathrm{vac}|\boldsymbol{Q}|\mathrm{vac}\rangle = \mathbf{:}\overline{\overline{Q}}\mathbf{:}$. *The vacuum expectation value of a string of particle-hole operators equals the sum of its complete contractions.*

Proof: From Wick's theorem (Thm 4.1) we have that $Q = \mathbf{:}Q\mathbf{:} + \mathbf{:}\overline{Q}\mathbf{:}$. Taking the vacuum expectation value of both sides gives $\langle \mathrm{vac}|Q|\mathrm{vac}\rangle = \mathbf{:}\overline{\overline{Q}}\mathbf{:}$ since all terms with incompletely contracted operators have vanishing vac expectation values.

Proposition 4.1. ***Sign rule for completely contracted products.*** *The phase factor of a completely contracted product is given by $(-)^c$ where c is the number of crossings between contraction lines.*

Proof: Let $\varepsilon_\pi \mathbf{:}\overbrace{q_{\pi(1)} q_{\pi(2)}} \cdots \overbrace{q_{\pi(2n-1)} q_{\pi(2n)}}\mathbf{:}$ be the disentangled form of a complete contraction of $q_1 \cdots q_{2n}$. The phase factor for the contraction, ε_π, is equal to the signature of the disentangling permutation, which is equal to the signature of its inverse ("re-entangling") permutation. Consider re-entangling the product by transpositions of adjacent operators, noting that we only need transpositions involving operator pairs which are not contracted with each other. Since every operator has a contraction line overhead, each transposition changes the number of crossings by exactly ± 1. Therefore, $\varepsilon_\pi = (-)^c$ where c is the number of crossings.

5 Φ-normal ordering

Remark 5.1. ***Hole-particle isomorphism.*** Let Φ, corresponding to the occupation vector $|\underset{n\text{ times}}{1\cdots1}000\cdots\rangle$, be a reference determinant and consider the mapping $F(\mathcal{H}) \to F(\mathcal{H})$ given by inverting the bits occupied in Φ:

$$|n_1\cdots n_n n_{n+1}n_{n+2}\cdots\rangle \mapsto |\overline{n}_1\cdots\overline{n}_n n_{n+1}n_{n+2}\cdots\rangle \text{ where } \overline{n}_i = 1 - n_i \ .$$

This mapping is invertible, so it defines an isomorphism. Physically, this corresponds to viewing the first n states as *hole states* rather than as *particle states*. Collectively, these are referred to as *quasiparticle states*. Under this isomorphism, $|\text{vac}\rangle \mapsto |\underset{n\text{ times}}{\overline{1}\cdots\overline{1}}000\cdots\rangle$ becomes a state of n holes and $|\Phi\rangle \mapsto |\underset{n\text{ times}}{\overline{0}\cdots\overline{0}}000\cdots\rangle$ becomes the *quasiparticle vacuum*, in which all hole and particle states are unoccupied.

Definition 5.1. ***Quasiparticle creation and annihilation operators.*** Let $\{b_p\} \cup \{b_p^\dagger\}$ be the *quasiparticle creation and annihilation operators* that result from applying the isomorphism discussed in Rmk 5.1. These are related to the original set $\{a_p\} \cup \{a_p^\dagger\}$ of *particle creation and annihilation operators* via

$$a_i \mapsto b_i^\dagger \qquad a_i^\dagger \mapsto b_i \qquad a_a \mapsto b_a \qquad a_a^\dagger \mapsto b_a^\dagger$$

where i and a are occupied and virtual indices with respect to Φ. $\{a_i^\dagger\} \cup \{a_a\} \mapsto \{b_p\}$ are therefore *quasiparticle annihilation operators* and $\{a_i\} \cup \{a_a^\dagger\} \mapsto \{b_p^\dagger\}$ are *quasiparticle creation operators*.

Definition 5.2. **Φ-*normal order.*** A string $q_1\cdots q_n$ of particle-hole operators $q_i \in \{a_p\} \cup \{a_p^\dagger\}$ is in Φ-*normal order* when all of its quasiparticle creation operators lie to the left of all of its quasiparticle annihilation operators. That is, it must map to a string of the form $b_{p_1}^\dagger \cdots b_{p_m}^\dagger b_{r_1} \cdots b_{r_{m'}}$ under the hole-particle isomorphism (Rmk 5.1) that makes Φ the quasiparticle vacuum. This quarantees that $\langle\Phi|q_1\cdots q_n|\Phi\rangle = 0$, i.e. its Φ expectation value vanishes.

Definition 5.3. **Φ-*normal ordering.*** The Φ-*normal ordering* of a string $q_1\cdots q_n$ of particle-hole operators is the mapping $q_1\cdots q_n \mapsto :q_1\cdots q_n: = \varepsilon_\pi q_{\pi(1)}\cdots q_{\pi(n)}$ where $\pi \in \mathrm{S}_n$ is a permutation that places the string in Φ-normal order.

Definition 5.4. **Φ-*normal contraction.*** A pairwise Φ-*normal contraction* $\overbracket{q_1 q_2}$ is defined as $\overbracket{q_1 q_2} \equiv q_1q_2 - :q_1q_2:$. For the quasiparticle operators of Def 5.1, the only non-vanishing contraction is $\overbracket{b_p b_q^\dagger} = \delta_{pq}$, which shows that $\overbracket{a_i^\dagger a_j} = \delta_{ij}$ and $\overbracket{a_a a_b^\dagger} = \delta_{ab}$ are the non-vanishing Φ-normal contractions of the orignal particle-hole operators.

Remark 5.2. ***Non-vanishing contractions are elements of the Φ one-particle and one-hole density matrices.*** Φ-normal contractions can in general be identified with $\overbracket{q_1 q_2} = \langle\Phi|q_1q_2 - :q_1q_2:|\Phi\rangle = \langle\Phi|q_1q_2|\Phi\rangle$. Therefore, the non-vanishing contractions are elements of the Φ one-particle and one-hole density matrices

$$\overbracket{a_p^\dagger a_q} = \langle\Phi|a_p^\dagger a_q|\Phi\rangle = \gamma_{qp} \qquad\qquad \overbracket{a_p a_q^\dagger} = \langle\Phi|a_p a_q^\dagger|\Phi\rangle = \eta_{pq}$$

depending whether the creation operator is on the right or left in the contraction. The one-particle density matrix of Φ is given by $\gamma_{pq} = 0$ unless $p = q = i$ where i is an occupied index, in which case $\gamma_{ii} = 1$. The one-hole density matrix of Φ is given by $\eta_{pq} = 0$ unless $p = q = a$ where a is a virtual index, in which case $\eta_{aa} = 1$.

Definition 5.5. **Φ-*normal ordering with contractions.*** If $q_1\cdots q_n$ is a string of particle-hole operators, its Φ-*normal ordering with contraction* $\overbracket{q_i q_j}$ $(i < j)$ is defined as $:q_1\cdots\overbracket{q_i\cdots q_j}\cdots q_n: \equiv (-)^{j-i-1}\overbracket{q_i q_j}:q_1\cdots\cancel{q_i}\cdots\cancel{q_j}\cdots q_n:$.

Remark 5.3. ***Wick's theorem for Φ-normal ordering.*** The isomorphism described in Rmk 5.1 maps Φ-normal ordered products with Φ-normal contractions into vac-normal ordered products with vac-normal contractions. Therefore, Wick's theorem still holds as $Q = :Q: + :\overline{Q}:$ with non-vanishing contractions $\overbracket{a_p^\dagger a_q} = \gamma_{qp}$ and $\overbracket{a_p a_q^\dagger} = \eta_{pq}$. The corollaries $:Q::Q': = :QQ': + :\overbracket{QQ'}:$ and $\langle\Phi|Q|\Phi\rangle = :\overline{\overline{Q}}:$ also still hold, since they follow directly from Wick's theorem.

Remark 5.4. As an example, consider the Φ-normal Wick expansion of $a_p^\dagger a_q$ and $a_p^\dagger a_q^\dagger a_s a_r$:

$$\begin{aligned}
a_p^\dagger a_q &= :a_p^\dagger a_q: + :\overbracket{a_p^\dagger a_q}: = :a_p^\dagger a_q: + \gamma_{qp} \\
a_p^\dagger a_q^\dagger a_s a_r &= :a_p^\dagger a_q^\dagger a_s a_r: + :\overbracket{a_p^\dagger a_q^\dagger} a_s a_r: + :\overbracket{a_p^\dagger a_q^\dagger a_s a_r}: + :a_p^\dagger \overbracket{a_q^\dagger a_s} a_r: + :a_p^\dagger a_q^\dagger \overbracket{a_s a_r}: + :\overbracket{a_p^\dagger a_q^\dagger a_s a_r}: + :\overbracket{a_p^\dagger \overbracket{a_q^\dagger a_s} a_r}: \\
&= :a_p^\dagger a_q^\dagger a_s a_r: - \gamma_{sp}:a_q^\dagger a_r: + \gamma_{rp}:a_q^\dagger a_s: + \gamma_{sq}:a_p^\dagger a_r: - \gamma_{rq}:a_p^\dagger a_s: + \gamma_{rp}\gamma_{sq} - \gamma_{sp}\gamma_{rq} \ .
\end{aligned}$$

In general, an m-tuple excitation operator $a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1}$ can be expressed as a linear combination of Φ-normal ordered n-tuple excitation operators $:a_{r_1}^\dagger \cdots a_{r_n}^\dagger a_{s_n} \cdots a_{s_1}:$ from $n = 0$ to $n = m$.

6 Kutzelnigg-Mukherjee tensor notation

Notation 6.1. ***Kutzelnigg-Mukherjee tensor notation.*** In *Kutzelnigg-Mukherjee tensor notation* (*KM notation*), indices which are covariant with respect to the spin-orbital basis $\{\psi_p\}$ are written as superscripts, whereas contravariant indices are written as subscripts. Note that this reverses the usual convention in multilinear algebra. Furthermore, the Einstein summation convention is adopted, in which any pair of matching upper and lower indices in a product is implicitly summed over its index range. Indices $i, j, k, l, \cdots$ count over occupied orbitals $\{\psi_i \in \Phi\}$, indices $a, b, c, d, \cdots$ count over virtual orbitals $\{\psi_a \notin \Phi\}$, and indices $p, q, r, s, \cdots$ count over the full spin-orbital basis $\{\psi_p \in \mathcal{H}\}$.

Notation 6.2. ***KM notation for particle-hole operators.*** Annihilation operators (a_p) are contravariant and creation operators ($a_p^\dagger$) operators are covariant to the spin-orbital basis, so these are written as a_p and a^p, respectively.

Notation 6.3. ***KM notation for one-hole and one-particle density matrices.*** The one-particle and one-hole density matrices of a state Ψ are written as $\gamma_q^p = \langle\Psi|a^p a_q|\Psi\rangle$ and $\eta_p^q = \langle\Psi|a_p a^q|\Psi\rangle$, respectively.

Notation 6.4. ***KM notation for excitation operators.*** Excitation operators are given the following concise notation.

$$a^{p_1\cdots p_m}_{q_1\cdots q_m} \equiv a^{p_1}\cdots a^{p_m} a_{q_m}\cdots a_{q_1}$$

Φ-normal-ordered excitation operators are denoted with a tilde: $\tilde{a}^{p_1\cdots p_m}_{q_1\cdots q_m} \equiv \{\!\{a^{p_1\cdots p_m}_{q_1\cdots q_m}\}\!\}$.

Notation 6.5. ***KM notation for H_e.*** The electronic Hamiltonian is expressed in KM notation as

$$H_e = h^q_p a^p_q + \tfrac{1}{2} g^{rs}_{pq} a^{pq}_{rs} \qquad \text{or} \qquad H_e = h^q_p a^p_q + \tfrac{1}{4}\overline{g}^{rs}_{pq} a^{pq}_{rs}$$

where $h^q_p \equiv \langle\psi_p(1)|\hat{h}(1)|\psi_q(1)\rangle$ are the one-electron integrals, $g^{rs}_{pq} \equiv \langle\psi_p(1)\psi_q(2)|\hat{g}(1,2)|\psi_r(1)\psi_s(2)\rangle$ are the two-electron integrals, and $\overline{g}^{rs}_{pq} \equiv g^{rs}_{pq} - g^{sr}_{pq}$ are the antisymmetrized two-electron integrals.

Remark 6.1. Note that for normal-ordered products of excitation operators, the following rearrangements are valid.

$$\{\!\{a^{p_1\cdots p_m}_{q_1\cdots q_m} a^{r_1\cdots r_n}_{s_1\cdots s_n}\}\!\} = \{\!\{a^{p_1}_{q_1}\cdots a^{p_m}_{p_m} a^{r_1}_{s_1}\cdots a^{r_n}_{s_n}\}\!\} = a^{p_1\cdots p_m r_1\cdots r_n}_{q_1\cdots q_m s_1\cdots s_n}$$
$$\{\!\{\tilde{a}^{p_1\cdots p_m}_{q_1\cdots q_m} \tilde{a}^{r_1\cdots r_n}_{s_1\cdots s_n}\}\!\} = \{\!\{\tilde{a}^{p_1}_{q_1}\cdots \tilde{a}^{p_m}_{p_m} \tilde{a}^{r_1}_{s_1}\cdots \tilde{a}^{r_n}_{s_n}\}\!\} = \tilde{a}^{p_1\cdots p_m r_1\cdots r_n}_{q_1\cdots q_m s_1\cdots s_n}$$

Furthermore, every one of these expressions is antisymmetric in its upper and lower indices – for example, $\{\!\{a^p_q a^{rs}_{tu}\}\!\} = -\{\!\{a^r_q a^{ps}_{tu}\}\!\} = \{\!\{a^r_t a^{ps}_{qu}\}\!\}$. The phase factor for permutations of upper or lower indices is $(-)^t$ where t is the number of transpositions required to restore the original pairing ($\begin{smallmatrix} p_i \\ q_i \end{smallmatrix}$ and $\begin{smallmatrix} r_i \\ s_i \end{smallmatrix}$) of upper and lower indices. When the pairs are permuted together, no change in sign appears: $a^{p_1\cdots p_m}_{q_1\cdots q_m} = a^{p_{\pi(1)}\cdots p_{\pi(m)}}_{q_{\pi(1)}\cdots q_{\pi(m)}}$ for all $\pi \in \mathrm{S}_m$.

Notation 6.6. ***Notation for contractions.*** It is convenient here to shift to the following notation for contractions

$$a_{p^\circ} a^{q^\circ} \equiv \overbrace{a_p a^q} \qquad a^{q^\circ} a_{p^\circ} \equiv -\overbrace{a_p a^q} \qquad a^{p^\bullet} a_{q^\bullet} \equiv \overbrace{a^p a_q} \qquad a_{q^\bullet} a^{p^\bullet} \equiv -\overbrace{a^p a_q}$$

where $\circ$ indicates an *η-contraction* and $\bullet$ indicates a *γ-contraction* between operators with the same number of these symbols next to their indices. Note that $a^{q^\circ}_{p^\circ} = -\eta^q_p$ ($= -\delta^q_p$ for a vac-normal contraction) and $a^{p^\bullet}_{q^\bullet} = \gamma^p_q$ ($= 0$ for a vac-normal contraction). This notation allows for contracted operators to be permuted arbitrarily with the other operators in a normal-ordered string, in contrast to $\overbrace{a_p a^q}$ and $\overbrace{a^p a_q}$ which are neither antisymmetric nor symmetric to interchange of their arguments.

Notation 6.7. ***Index permutation operators.*** Let $\hat{P}^{(P_1/\cdots/P_M)}_{(Q_1/\cdots/Q_N)}$, where P_i and Q_i are sets of indices, denote an *index permutation operator* which yields a sum over all permutations of the indices in $P_1\cdots P_M$ and $Q_1\cdots Q_M$ weighted by the permutation phases, omitting any permutations that involve transpositions within one of the blocks, P_i or Q_i.

Remark 6.2. Repeating the examples from Rmk 5.4 using KM notation, we write

$$a^p_q = \{\!\{a^p_q\}\!\} + \{\!\{a^{p^\bullet}_{q^\bullet}\}\!\} \qquad = \tilde{a}^p_q + \gamma^p_q$$
$$a^{pq}_{rs} = \{\!\{a^{pq}_{rs}\}\!\} + \{\!\{a^{p^\bullet q}_{r^\bullet s}\}\!\} + \{\!\{a^{p^\bullet q}_{rs^\bullet}\}\!\} + \{\!\{a^{pq^\bullet}_{r^\bullet s}\}\!\} + \{\!\{a^{pq^\bullet}_{rs^\bullet}\}\!\} + \{\!\{a^{p^\bullet q^{\bullet\bullet}}_{r^\bullet s^{\bullet\bullet}}\}\!\} + \{\!\{a^{p^\bullet q^{\bullet\bullet}}_{r^{\bullet\bullet} s^\bullet}\}\!\} \qquad = \tilde{a}^{pq}_{rs} + \hat{P}^{(p/q)}_{(r/s)} \tilde{a}^q_s \gamma^p_r + \hat{P}_{(r/s)} \gamma^p_r \gamma^q_s$$

where $\hat{P}_{(r/s)}$ acts as $\hat{P}_{(r/s)} f_{rs} = f_{rs} - f_{sr}$ and $\hat{P}^{(p/q)}_{(r/s)}$ acts as $\hat{P}^{(p/q)}_{(r/s)} f^{pq}_{rs} = \hat{P}^{(p/q)} \hat{P}_{(r/s)} f^{pq}_{rs} = f^{pq}_{rs} - f^{pq}_{sr} - f^{qp}_{rs} + f^{qp}_{sr}$. More complicated permutation operators appear in the Φ-normal Wick expansions of higher excitation operators, such as

$$a^{pqr}_{stu} = \tilde{a}^{pqr}_{stu} + \hat{P}^{(p/qr)}_{(s/tu)} \gamma^p_s \tilde{a}^{qr}_{tu} + \hat{P}^{(pq/r)}_{(s/t/u)} \gamma^p_s \gamma^q_r \tilde{a}^r_u + \hat{P}_{(s/t/u)} \gamma^p_s \gamma^q_t \gamma^r_u$$

Where $\hat{P}_{(p/q/r)}$ sums over all permutations of pqr: $\hat{P}_{(p/q/r)} f_{pqr} = f_{pqr} - f_{prq} - f_{qpr} + f_{qrp} + f_{rpq} - f_{rqp}$, whereas $\hat{P}_{(p/qr)}$ omits any permutations that involve transpose q and r: $\hat{P}_{(p/qr)} f_{pqr} = f_{pqr} - f_{qpr} - f_{rqp}$.

Remark 6.3. The Wick expansions for a^p_q and a^{pq}_{rs} can be used to write $H_e = h^q_p a^p_q + g^{rs}_{pq} a^{pq}_{rs}$ as

$$H_e = \langle \Phi | H_e | \Phi \rangle + f^q_p \tilde{a}^p_q + \tfrac{1}{4} \overline{g}^{rs}_{pq} \tilde{a}^{pq}_{rs}$$

where $\langle \Phi | H_e | \Phi \rangle = h^q_p \gamma^p_q + \frac{1}{2} \overline{g}^{rs}_{pq} \gamma^p_r \gamma^q_s = h^i_i + \frac{1}{2} \overline{g}^{ij}_{ij}$ is the Hartree-Fock energy expression and $f^q_p = h^q_p + \overline{g}^{qs}_{pr} \gamma^r_s = h^q_p + \overline{g}^{qi}_{pi}$ is the spin-orbital Fock matrix.

Remark 6.4. ***Example: Derivation of Slater-Condon rules in KM notation.*** Noting $a^{abc\cdots}_{ijk\cdots} = \tilde{a}^{abc\cdots}_{ijk\cdots}$ since these excitation operators consist of only quasiparticle creation operators, Hamiltonian matrix elements $\langle \Phi | H_e | \Phi^{abc\cdots}_{ijk\cdots} \rangle$ can be evaluated from $\langle \Phi | \tilde{a}^p_q \tilde{a}^{abc\cdots}_{ijk\cdots} | \Phi \rangle$ and $\langle \Phi | \tilde{a}^{pq}_{rs} \tilde{a}^{abc\cdots}_{ijk\cdots} | \Phi \rangle$. According to Wick's theorem, $\langle \Phi | \tilde{a}^p_q \tilde{a}^{abc\cdots}_{ijk\cdots} | \Phi \rangle$ is equal to the complete cross-contractions between $\tilde{a}^p_q$ and $\tilde{a}^{abc\cdots}_{ijk\cdots}$, so that these matrix elements are as follows.

$$\langle \Phi | \tilde{a}^p_q | \Phi \rangle = 0$$
$$\langle \Phi | \tilde{a}^p_q \tilde{a}^a_i | \Phi \rangle = \colon a^{p^\bullet}_{q^\circ} a^{a^\circ}_{i^\bullet} \colon = \gamma^p_i \eta^a_q$$
$$\langle \Phi | \tilde{a}^p_q \tilde{a}^{ab}_{ij} | \Phi \rangle = 0$$

Beyond single excitations, the matrix elements vanish because there are no possible complete cross-contractions. Similarly, $\langle \Phi | \tilde{a}^{pq}_{rs} \tilde{a}^{abc\cdots}_{ijk\cdots} | \Phi \rangle$ is equal to the sum over complete cross-contractions between $\tilde{a}^{pq}_{rs}$ and $\tilde{a}^{abc\cdots}_{ijk\cdots}$.

$$\langle \Phi | \tilde{a}^{pq}_{rs} | \Phi \rangle = 0$$
$$\langle \Phi | \tilde{a}^{pq}_{rs} \tilde{a}^a_i | \Phi \rangle = 0$$
$$\langle \Phi | \tilde{a}^{pq}_{rs} \tilde{a}^{ab}_{ij} | \Phi \rangle = \colon a^{p^\bullet q^{\bullet\bullet}}_{r^\circ s^{\circ\circ}} a^{a^\circ b^{\circ\circ}}_{i^\bullet j^{\bullet\bullet}} \colon + \colon a^{p^\bullet q^{\bullet\bullet}}_{r^\circ s^{\circ\circ}} a^{a^{\circ\circ} b^\circ}_{i^{\bullet\bullet} j^\bullet} \colon + \colon a^{p^\bullet q^{\bullet\bullet}}_{r^\circ s^{\circ\circ}} a^{a^{\circ\circ} b^{\circ\circ}}_{i^\bullet j^\bullet} \colon + \colon a^{p^\bullet q^{\bullet\bullet}}_{r^\circ s^{\circ\circ}} a^{a^{\circ\circ} b^\circ}_{i^{\bullet\bullet} j^\bullet} \colon = \hat{P}^{(a/b)}_{(i/j)} \gamma^p_i \gamma^q_j \eta^a_r \eta^b_s$$
$$\langle \Phi | \tilde{a}^{pq}_{rs} \tilde{a}^{abc\cdots}_{ijk\cdots} | \Phi \rangle = 0$$

Beyond double excitations, no complete cross-contractions are possible and the matrix elements vanish. Using these results, the first Slater-Condon rule becomes tautological: $\langle \Phi | H_e | \Phi \rangle + f^q_p \langle \Phi | \tilde{a}^p_q | \Phi \rangle + \frac{1}{4} \overline{g}^{rs}_{pq} \langle \Phi | \tilde{a}^{pq}_{rs} | \Phi \rangle = \langle \Phi | H_e | \Phi \rangle$. The remaining Slater-Condon rules take the following form.

$$\langle \Phi | H_e | \Phi^a_i \rangle = f^q_p \gamma^p_i \eta^a_q = f^i_a \qquad \langle \Phi | H_e | \Phi^{ab}_{ij} \rangle = \tfrac{1}{4} \overline{g}^{rs}_{pq} \left(\hat{P}^{(a/b)}_{(i/j)} \gamma^p_i \gamma^q_j \eta^a_r \eta^b_s \right) = \overline{g}^{ab}_{ij} \qquad \langle \Phi | H_e | \Phi^{abc\cdots}_{ijk\cdots} \rangle = 0$$

More general matrix elements $\langle \Phi^A_I | H_e | \Phi^B_J \rangle$ can be evaluated similarly by determining the complete cross-contractions of $\tilde{a}^I_A \tilde{a}^p_q \tilde{a}^B_J$ and $\tilde{a}^I_A \tilde{a}^{pq}_{rs} \tilde{a}^B_J$.

Definition 6.1. ***Φ-normal electronic Hamiltonian.*** The Φ-*normal electronic Hamiltonian*, here denoted H_c, is defined as $H_c \equiv H_e - \langle \Phi | H_e | \Phi \rangle$. Using Rmk 6.3, it can be expressed as follows.

$$H_c = f^q_p \tilde{a}^p_q + \tfrac{1}{4} \overline{g}^{rs}_{pq} \tilde{a}^{pq}_{rs}$$

H_c shares the same eigenstates as H_e, but it has a vanishing Φ expectation value and its eigenvalues are correlation energies $E_c = E_e - \langle \Phi | H_e | \Phi \rangle$ with respect to Φ.

Remark 6.5. ***Example: Derivation of CI singles equations in KM notation.*** The eigenvalue-shifted CI singles matrix $\langle \Phi^a_i | H_e | \Phi^b_j \rangle - \langle \Phi | H_e | \Phi \rangle \delta_{ij} \delta^{ab}$ is equivalent to $\langle \Phi^a_i | H_c | \Phi^b_j \rangle$. Its matrix elements can be determined from

$$\langle \Phi | \tilde{a}^i_a \tilde{a}^p_q \tilde{a}^b_j | \Phi \rangle = \colon a^{i^\bullet}_{a^\circ} a^{p^\circ}_{q^{\circ\circ}} a^{b^{\circ\circ}}_{j^\bullet} \colon + \colon a^{i^\bullet}_{a^\circ} a^{p^{\bullet\bullet}}_{q^\bullet} a^{b^\circ}_{j^{\bullet\bullet}} \colon = \gamma^i_j \eta^p_a \eta^b_q - \gamma^i_q \gamma^p_j \eta^b_a$$
$$\langle \Phi | \tilde{a}^i_a \tilde{a}^{pq}_{rs} \tilde{a}^b_j | \Phi \rangle = \colon \tilde{a}^{i^\bullet}_{a^\circ} \tilde{a}^{p^\circ q^{\bullet\bullet}}_{r^\bullet s^{\circ\circ}} \tilde{a}^{b^{\circ\circ}}_{j^{\bullet\bullet}} \colon + \colon \tilde{a}^{i^\bullet}_{a^\circ} \tilde{a}^{p^\circ q^{\bullet\bullet}}_{r^{\circ\circ} s^\bullet} \tilde{a}^{b^{\circ\circ}}_{j^{\bullet\bullet}} \colon + \colon \tilde{a}^{i^\bullet}_{a^\circ} \tilde{a}^{p^{\bullet\bullet} q^\circ}_{r^\bullet s^{\circ\circ}} \tilde{a}^{b^{\circ\circ}}_{j^{\bullet\bullet}} \colon + \colon \tilde{a}^{i^\bullet}_{a^\circ} \tilde{a}^{p^{\bullet\bullet} q^\circ}_{r^{\circ\circ} s^\bullet} \tilde{a}^{b^{\circ\circ}}_{j^{\bullet\bullet}} \colon = \hat{P}^{(p/q)}_{(r/s)} \gamma^i_r \eta^p_a \gamma^q_j \eta^b_s$$

which gives

$$\langle \Phi^a_i | H_c | \Phi^b_j \rangle = f^q_p \left(\gamma^i_j \eta^p_a \eta^b_q - \gamma^i_q \gamma^p_j \eta^b_a \right) + \tfrac{1}{4} \overline{g}^{rs}_{pq} \left(\hat{P}^{(p/q)}_{(r/s)} \gamma^i_r \eta^p_a \gamma^q_j \eta^b_s \right) = f^b_a \gamma^i_j - f^i_j \eta^b_a + \overline{g}^{ib}_{aj} \ .$$

Noting that $\gamma^i_j = \delta^i_j$ and $\eta^b_a = \delta^b_a$ (see Rmk 5.2), this can be simplified to $\langle \Phi^a_i | H_c | \Phi^b_j \rangle = f^b_a \delta^i_j - f^i_j \delta^b_a + \overline{g}^{ib}_{aj}$.

A Derivation of the pull-through relation

Proposition A.1. ***Pull-through relation.*** *For arbitrary operators $x_1, \ldots, x_n$ and y,*

$$x_1 \cdots x_n y = (\mp)^n y x_1 \cdots x_n + \sum_{k=1}^{n} (\mp)^{n-k} x_1 \cdots [x_k, y]_{\pm} \cdots x_n$$

where $[x, y]_{\pm} \equiv xy \pm yx$.

Proof: The $n = 1$ case follows from the definition of the commutator brackets: $xy = \mp yx + [x, y]_{\pm}$. Now, assume it holds for n and consider $n + 1$. Since $x_1 \cdots x_{n+1} y = x_1 \cdots x_n (\mp y x_{n+1} + [x_{n+1}, y]_{\pm})$, we find

$$\begin{aligned} x_1 \cdots x_{n+1} y = & \mp \left((\mp)^n y x_1 \cdots x_n + \sum_{k=1}^{n} (\mp)^{n-k} x_1 \cdots [x_k, y]_{\pm} \cdots x_n \right) x_{n+1} + x_1 \cdots x_n [x_{n+1}, y]_{\pm} \\ & = (\mp)^{n+1} y x_1 \cdots x_n + \sum_{k=1}^{n+1} (\mp)^{n+1-k} x_1 \cdots [x_k, y]_{\pm} \cdots x_{n+1} \end{aligned}$$

and, by induction, the result holds for all n.