Algebraic and Diagrammatic Methods in Electronic Structure Theory

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1. Fock space

1.1   Position-space representation

Definition 1.1. *n-electron Hilbert space.* If $\mathcal{H}$ is a complete one-electron Hilbert space and $\{\psi_p\}$ is its spin-orbital basis, then $\mathcal{H}^{\otimes n} = \mathcal{H} \underset{n \text{ times}}{\otimes \cdots \otimes} \mathcal{H} = \text{span}\{\psi_{p_1} \otimes \cdots \otimes \psi_{p_n}\}$ is an *n-electron Hilbert space*.[1] The inner product on $\mathcal{H}^{\otimes n}$ is

$$\langle \psi_{p_1} \otimes \cdots \otimes \psi_{p_n} | \psi_{q_1} \otimes \cdots \otimes \psi_{q_n} \rangle = \langle \psi_{p_1} | \psi_{q_1} \rangle \cdots \langle \psi_{p_n} | \psi_{q_n} \rangle. \tag{1.1}$$

Projection onto $\langle 1 \otimes \cdots \otimes n |$, where $|i\rangle = |\mathbf{r}_i, s_i\rangle$ is a space-spin electronic state, reveals that the basis states $\psi_{p_1} \otimes \cdots \otimes \psi_{p_n}$ are abstact representations of ordinary product states, $\langle 1 \otimes \cdots \otimes n | \psi_{p_1} \otimes \cdots \otimes \psi_{p_n} \rangle = \psi_{p_1}(1) \cdots \psi_{p_n}(n)$.

Definition 1.2. *n-electron Slater determinant.* An *n-electron Slater determinant* $\Phi_{(p_1 \cdots p_n)}$ is a normalized antisymmetric product of n one-electron states $\psi_{p_1}, \cdots, \psi_{p_n}$

$$\Phi_{(p_1 \cdots p_n)} = \frac{1}{\sqrt{n!}} \sum_{\pi \in S_n} \varepsilon_\pi \psi_{p_{\pi(1)}} \otimes \cdots \otimes \psi_{p_{\pi(n)}} \tag{1.2}$$

where $\pi \in S_n$ is a permutation of $1 \cdots n$ and ε_π is $(-)^{\# \text{ transpositions}}$. Projecting into position space yields its familiar form.

$$\langle 1 \otimes \cdots \otimes n | \Phi_{(p_1 \cdots p_n)} \rangle = \Phi_{(p_1 \cdots p_n)}(1, \cdots, n) = \frac{1}{\sqrt{n!}} \det |\psi_{p_{\pi(1)}}(1) \cdots \psi_{p_{\pi(n)}}(n)|$$

Remark 1.1. *A direct derivation of second quantization in position-space representation.* Let F_n be the space of n-electron Slater determinants, $\Phi_{(p_1 \cdots p_n)}$, a subspace of $\mathcal{H}^{\otimes n}$. Consider the integral operator $\hat{a}_p : F_n \to F_{n-1}$ given by

$$\Psi(1, \cdots, n) \mapsto (\hat{a}_p \Psi)(2, \cdots, n) \equiv \sqrt{n} \int d(1) \psi_p^*(1) \Psi(1, 2, \cdots, n). \tag{1.3}$$

This operator acts on Slater determinants as

$$(\hat{a}_p \Phi_{(p_1 \cdots p_n)})(2, \cdots, n) = \frac{1}{\sqrt{(n-1)!}} \sum_{\pi \in S_n} \langle \psi_p | \psi_{p_{\pi(1)}} \rangle \psi_{p_{\pi(2)}}(2) \cdots \psi_{p_{\pi(n)}}(n) = \begin{cases} (-)^{k-1} \Phi_{(p_1 \cdots \not{p_k} \cdots p_n)} & p = p_k \in (p_1 \cdots p_n) \\ 0 & \text{otherwise} \end{cases}$$

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[1] See def A.6 for the definition of a tensor product.

i.e. it deletes the orbital ψ_p from $\Phi_{(p_1\cdots p_n)}$ if exists and otherwise kills the determinant. The restriction of $\hat{a}_p$ to the space of antisymmetric functions implies that these operators anticommute, $\hat{a}_p\hat{a}_q = -\hat{a}_q\hat{a}_p$, since

$$\int d(1)d(2)\psi_p^*(1)\psi_q^*(2)\Psi(1,2,\cdots,n) = \int d(1)d(2)\psi_q^*(1)\psi_p^*(2)\Psi(2,1,\cdots,n) = -\int d(1)d(2)\psi_q^*(1)\psi_p^*(2)\Psi(1,2,\cdots,n)$$

by changing dummy variables of integration and plugging in $\Psi(2,1,\cdots,n) = -\Psi(1,2,\cdots,n)$. These deletion operators provide the following decomposition of functions in F_n.

$$\Psi(1,\cdots,n) = \tfrac{1}{\sqrt{n}}\sum_p^\infty \psi_p(1)\,(\hat{a}_p\Psi)\,(2,\cdots,n) = \tfrac{1}{\sqrt{n(n-1)}}\sum_{pq}^\infty \psi_p(1)\psi_q(2)(\hat{a}_q\hat{a}_p\Psi)(3,\cdots,n) \tag{1.4}$$

Therefore, general matrix elements of the electronic Hamiltonian with respect to $\Psi,\Psi' \in F_n$ can be expressed as

$$\langle\Psi|\hat{H}_e\Psi'\rangle = \sum_{i=1}^n \langle\Psi|\hat{h}(i)\Psi'\rangle + \sum_{i<j}^n \langle\Psi|\hat{g}(i,j)\Psi'\rangle = n\langle\Psi|\hat{h}(1)\Psi'\rangle + \tfrac{n(n-1)}{2}\langle\Psi|\hat{g}(1,2)\Psi'\rangle$$

$$= \sum_{pq}^\infty h_{pq}\langle\hat{a}_p\Psi|\hat{a}_q\Psi'\rangle + \tfrac{1}{2}\sum_{pqrs}^\infty \langle pq|rs\rangle\langle\hat{a}_q\hat{a}_p\Psi|\hat{a}_s\hat{a}_r\Psi'\rangle$$

where $\hat{h}(i) \equiv -\tfrac{1}{2}\nabla_i^2 + \sum_A \frac{Z_A}{|\mathbf{r}_i - \mathbf{R}_A|}$, $\hat{g}(i,j) \equiv \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$, $h_{pq} \equiv \langle\psi_p(1)|\hat{h}(1)\psi_q(1)\rangle$, and $\langle pq|rs\rangle \equiv \langle\psi_p(1)\psi_q(2)|\hat{g}(1,2)\psi_r(1)\psi_s(2)\rangle$. Therefore, restricting $\hat{H}_e$ to the space of physically realistic (i.e. antisymmetric) functions, we get the following identity

$$\hat{H}_e = \sum_{pq}^\infty h_{pq}\hat{a}_p^\dagger\hat{a}_q + \tfrac{1}{2}\sum_{pqrs}^\infty \langle pq|rs\rangle\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_s\hat{a}_r \tag{1.5}$$

which is the *second quantized* form of the Hamiltonian, as opposed to the *first quantized* form which is not restricted to antisymmetric functions. A defining feature of the second quantization formalism is that $\hat{H}_e$ is independent of the number of electrons.

1.2 Abstract representation

Definition 1.3. *Fock space.* Let $F_n(\mathcal{H})$ denote span$\{\Phi_{(p_1\cdots p_n)}\}$, the antisymmetric subspace of $\mathcal{H}^{\otimes n}$. The fermionic *Fock space* is the union of all of these spaces, $F(\mathcal{H}) = F_0(\mathcal{H}) \oplus F_1(\mathcal{H}) \oplus F_2(\mathcal{H}) \oplus \cdots \oplus F_\infty(\mathcal{H})$, which comprises all possible electronic wavefunctions.

Definition 1.4. *The occupation number representation of $F(\mathcal{H})$.* In the *occupation number representation* of Fock space, the basis vectors are represented as lists of 1s and 0s, $|\mathbf{n}\rangle \equiv |n_1, n_2, n_3, \cdots, n_\infty\rangle$, where $n_p = 1$ when ψ_p is occupied and $n_p = 0$ when ψ_p is unoccupied in the state. One possible basis for $F(\mathcal{H})$ is given by distributing 1s and 0s over the occupation vector in all possible ways. The state in which no spin-orbitals are occupied is called the *vacuum state*, denoted $|\text{vac}\rangle$, which spans $F_0(\mathcal{H}) \simeq \mathbb{C}$.

Definition 1.5. *Particle-hole operators.* *Particle-hole operators* change the occupation numbers of one-particle states. The *annihilation operator* of ψ_p is a linear mapping $a_p : F_n(\mathcal{H}) \to F_{n-1}(\mathcal{H})$ defined by

$$a_p|\cdots n_p\cdots\rangle = (-)^{n_1+\cdots+n_{p-1}}|\cdots n_p - 1\cdots\rangle \quad \text{if } n_p = 1 \qquad\qquad a_p|\cdots n_p\cdots\rangle = 0 \quad \text{if } n_p = 0 \tag{1.6}$$

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

$$c_p|\cdots n_p\cdots\rangle = (-)^{n_1+\cdots+n_{p-1}}|\cdots n_p + 1\cdots\rangle \quad \text{if } n_p = 0 \qquad\qquad c_p|\cdots n_p\cdots\rangle = 0 \quad \text{if } n_p = 1. \tag{1.7}$$

Proposition 1.1. $c_p = a_p^\dagger$. *Creation and annihilation operators of the same 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 $n_q' = n_q\ \forall q \neq p$. Likewise 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 all $\Psi, \Psi' \in F(\mathcal{H})$ and $c_p = a_p^\dagger$ by the definition of adjoint.

Proposition 1.2. $[q, q']_+ = \delta_{q'q^\dagger}$. *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 ψ_p and $\psi_{p'}$, respectively. First, suppose $p \neq p'$. Then

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

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

where $\overline{n_p}$ and $\overline{n_{p'}}$ are the occupations after applying q and q'. Since n_p and $\overline{n_p}$ differ by one, $qq' = -q'q$. The second case, $p = p'$, implies $q' \in \{q, q^\dagger\}$. If $q' = q$, then $qq' = -q'q = 0$. If $q' = q^\dagger$, either $n_p = 1 \implies (a_p^\dagger a_p + a_p a_p^\dagger) | \cdots n_p \cdots \rangle = (1+0) | \cdots n_p \cdots \rangle$ or $n_p = 0 \implies (a_p^\dagger a_p + a_p a_p^\dagger) | \cdots n_p \cdots \rangle = (0+1) | \cdots n_p \cdots \rangle$. Either way, $q' = q^\dagger \implies (qq' + q'q) = 1$.

Remark 1.2. *Relating the determinant and occupation number representations.* When $p_1 < \cdots < p_n$, $\Phi_{(p_1 \cdots p_n)}$ is equivalent to the occupation vector $|\mathbf{n}_{(p_1 \cdots p_n)}\rangle$ with 1s at $p_1, \cdots, p_n$. Otherwise, this determinant is equivalent to $\varepsilon_\pi |\mathbf{n}_{(p_1 \cdots p_n)}\rangle$ 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

$$a_p \Phi_{(p_1 \cdots p_n)} = (-)^{k-1} \Phi_{(p_1 \cdots \not{p_k} \cdots p_n)} \text{ if } p = p_k \in (p_1 \cdots p_n) \qquad a_p \Phi_{(p_1 \cdots p_n)} = 0 \text{ if } p \notin (p_1 \cdots p_n) \qquad (1.8)$$

$$a_p^\dagger \Phi_{(p_1 \cdots p_n)} = (-)^{k-1} \Phi_{(p_1 \cdots p_{k-1} p p_k \cdots p_n)} \text{ if } p \notin (p_1 \cdots p_n) \qquad a_p^\dagger \Phi_{(p_1 \cdots p_n)} = 0 \text{ if } p \in (p_1 \cdots p_n) \qquad (1.9)$$

which follows directly from eqs (1.6) and (1.7) when $p_1 < \cdots < p_n$. Other cases follow from the fact that any sign factors for permuting $(p_1 \cdots p_n)$ cancel on both sides of the equation, including the position of insertion or deletion, p_k, whose phase is tracked by $(-)^{k-1}$ on the right. That is, both sides of the equation are antisymmetric to permutations of $(1 \cdots n)$. Note that eq (1.8) was also derived in rmk 1.1 using the position-space representation of a_p. One advantage of the determinant basis is that, unlike occupation vectors, determinants translate directly into strings of creations operators

$$|\Phi_{(p_1 \cdots p_n)}\rangle = a_{p_1}^\dagger \cdots a_{p_n}^\dagger |\mathrm{vac}\rangle \qquad (1.10)$$

without any phase ambiguity. Together with the second quantized form of the electronic Hamiltonian (eq (1.5)), this boils much of the grunt work of electronic structure theory down to particle-hole operator algebra.

Definition 1.6. *Excitation operators and excited determinants.* Operator strings of the form $a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1}$ are called *excitation operators*. For a given reference determinant Φ, excited determinants can be constructed as

$$\Phi_{i_1 \cdots i_m}^{a_1 \cdots a_m} = a_{a_1}^\dagger \cdots a_{a_m}^\dagger a_{i_m} \cdots a_{i_1} \Phi = a_{a_1}^\dagger a_{i_1} \cdots a_{a_m}^\dagger a_{i_m} \Phi \qquad (1.11)$$

where $i_1, \cdots, i_m$ are occupied and $a_1, \cdots, a_m$ are virtual indices with respect to Φ.

2. vac-normal ordering

Definition 2.1. vac-*normal order.* A string $q_1 \cdots q_n$ of particle-hole operators is in vac-*normal order* when all of its creation operators sit to the left of its annihilation operators. That is, a vac-normal string has the form $a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{r_1} \cdots q_{r_{m'}}$. This form guarantees that the vacuum expectation value of the string goes to zero, $\langle \mathrm{vac}|q_1 \cdots q_n|\mathrm{vac}\rangle = 0$.

Definition 2.2. 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 2.3. vac-*normal contraction.* A vac-*normal contraction* of two particle particle-hole operators q_1 and q_2 is defined as $\overgroup{q_1 q_2} \equiv q_1 q_2 - \ :q_1 q_2:$. This associates a scalar value with every pair in $\{a_p\} \cup \{a_p^\dagger\}$, of which only $\overgroup{a_p a_q^\dagger} = a_p a_q^\dagger - \ :a_p a_q: \ = [a_p, a_q^\dagger]_+ = \delta_{pq}$ is non-zero.

Definition 2.4. n^{th} *order density moments.* The mth *order density moment* of a series of particle-hole operators $q_1, \cdots, q_m$ is the statistical average of their product, $\langle \Psi|q_1 \cdots q_m|\Psi\rangle$, with respect to a reference state $\Psi \in F(\mathcal{H})$.

Definition 2.5. *One-particle and one-hole density matrices.* For a state $\Psi \in F_n(\mathcal{H})$ with a definite particle count, the lowest-order non-vanishing density moments are $\gamma_{pq} \equiv \langle \Psi|a_q^\dagger a_p|\Psi\rangle$ and $\eta_{pq} \equiv \langle \Psi|a_p a_q^\dagger|\Psi\rangle$, the *one-particle* and *one-hole density matrices*.

Remark 2.1. vac-*normal contractions as pairwise density moments of the vacuum.* vac-normal contractions can be identified with pairwise moments of the vacuum state via $\overgroup{q_1 q_2} = \langle \mathrm{vac}|q_1 q_2 - \ :q_1 q_2:|\mathrm{vac}\rangle = \langle \mathrm{vac}|q_1 q_2|\mathrm{vac}\rangle$, since $\langle \mathrm{vac}|:q_1 q_2:|\mathrm{vac}\rangle = 0$ by definition and $\overgroup{q_2 q_2}$ is a scalar quantity. The only non-vanishing vac-normal contractions are elements of the vac one-hole density matrix, $\overgroup{a_p a_q^\dagger} = \langle \mathrm{vac}|a_p a_q^\dagger|\mathrm{vac}\rangle = \eta_{pq}$, which evaluates to δ_{pq}.

Notation 2.1. vac-*normal-ordered strings with contraction lines.* Let the notation $:q_1 \cdots \overline{q_i \cdots q_j} \cdots q_n:$ stand for

$$:q_1 \cdots \overline{q_i \cdots q_j} \cdots q_n: \equiv (-)^{j-i-1} \overline{q_i q_j} :q_1 \cdots \cancel{q_i} \cdots \cancel{q_j} \cdots q_n: \tag{2.1}$$

where the phase factor corresponds to the signature of the permutation required to join q_i and q_j. The same rule applies for vac-normal-ordered strings with multiple contraction lines.

Problem 2.1. Using only the anticommutator relation of prop 1.2, show that $a_p a_q a_s^\dagger a_r^\dagger$ can be expanded into the following linear combination of operator vac-normal operator strings.

$$a_p a_q a_s^\dagger a_r^\dagger = a_s^\dagger a_r^\dagger a_p a_q + \delta_{ps} a_r^\dagger a_q - \delta_{pr} a_s^\dagger a_q - \delta_{qs} a_r^\dagger a_p + \delta_{qr} a_s^\dagger a_p - \delta_{ps}\delta_{qr} + \delta_{pr}\delta_{qs}$$

and then show that the result can also be expressed as follows.

$$a_p a_q a_s^\dagger a_r^\dagger = :a_p a_q a_s^\dagger a_r^\dagger: + :\overline{a_p a_q} a_s^\dagger a_r^\dagger: + :\overline{a_p} a_q a_s^\dagger \overline{a_r^\dagger}: + :a_p \overline{a_q a_s^\dagger} a_r^\dagger: + :a_p \overline{a_q} a_s^\dagger \overline{a_r^\dagger}: + :\overline{a_p} \overline{a_q a_s^\dagger} a_r^\dagger: + :\overline{a_p} \overline{a_q} a_s^\dagger a_r^\dagger:$$

Notation 2.2. For a particle-hole operator string $Q = q_1 \cdots q_n$, let the $:Q(\overline{q_i q_j}):$ denote $:q_1 \cdots \overline{q_i \cdots q_j} \cdots q_n:$. This is well-defined as long as $i < j$. Let $:\overline{Q}:$ stand for the sum of all unique single, double, triple, etc. contractions of Q

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

where $\mathrm{Ctr}_k(Q)$ runs over all unique sets $\{(i_1 j_2) \cdots (i_k j_k) \,|\, i_p < j_p\}$ of k pairs of operator indices in Q and $\lfloor \cdot \rfloor$ is the floor function. Let $:\overline{\overline{Q}}:$ denote the sum of all *complete contractions*: the terms, if any, from $:\overline{Q}:$ in which every operator in Q is involved in a contraction. Finally, let $:\overline{QQ'}:$ denote the sum of all single, double, etc. *cross contractions*: those in which all contractions have an operator from Q on the left and one from Q' on the right. In this context, contractions involving two operators from Q or two operators from Q' are called *internal contractions* of Q or Q'.

Remark 2.2. Note that, using notation 2.2, the result of prob 2.1 can be expressed as $a_p a_q a_s^\dagger a_r^\dagger = :a_p a_q a_s^\dagger a_r^\dagger: + :\overline{a_p a_q a_s^\dagger a_r^\dagger}:$. This is a particular case of a more general result known as Wick's theorem, which says that any operator string Q is equal to its normal ordering plus the sum of all of its normal ordered contractions: $Q = :Q: + :\overline{Q}:$. The proof of this result follows in the next section (lem 2.1 and thm 2.1).

2.1 Wick's theorem

Lemma 2.1. $:Q:q = :Qq: + \sum_k :Q(\overline{q_k})q:$.
    Proof: Let n be the number of operators in Q and assume, without loss of generality, that Q is already in normal order so that $:Q: = Q$. If q is an annihilation operator then $:Qq: = Qq$ and all cross-contractions vanish, so the statement holds trivially. If q is a creation operator then $:Qq: = (-)^n qQ$ and, using the anticommutator relation from prop B.1,

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

since $:Q(\overline{q_k})q: = (-)^{n-k} q_1 \cdots \overline{q_k q} \cdots q_n$ and $\overline{q_k q} = [q_k, q]_+$ when q is a creation operator (see def 2.3).

Theorem 2.1. *Wick's theorem (time-independent).* $Q = :Q: + :\overline{Q}:$
    Proof: Let n be the length of Q. The result holds for $n = 2$ since $q_1 q_2 = :q_1 q_2: + \overline{q_1 q_2}$ by the definition of contraction (def 2.3). Now, assume it holds for n operators and consider Qq. By our inductive assumption, $Qq = :Q:q + :\overline{Q}:q$. Applying lem 2.1 to $:Q:q$ gives $:Q:q = :Qq: + \sum_i :Q(\overline{q_i})q:$. Expanding $:\overline{Q}:q$ and applying lem 2.1 to each term gives

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

$$= \sum_{(i_1 j_1)}^{\mathrm{Ctr}_1(Q)} :Q(\overline{q_{i_1} q_{j_1}})q: + \sum_{k=2}^{\lfloor (n+1)/2 \rfloor} \sum_{(i_1 j_2) \cdots (i_k j_k)}^{\mathrm{Ctr}_k(Qq)} :Qq(\overline{q_{i_1} q_{j_1}} \cdots \overline{q_{i_k} q_{j_k}}):$$

and, combining these results, we find

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$$Qq = :Q:q + :\overline{Q}:q = \quad :Qq: + \sum_{i=1}^{n} :Q(\overline{q_i)q}: + \sum_{(i_1 j_1)}^{\mathrm{Ctr}_1(Q)} :Q(\overline{q_{i_1}q_{j_1}})q: + \sum_{k=2}^{\lfloor (n+1)/2 \rfloor} \sum_{(i_1 j_2)\cdots(i_k j_k)}^{\mathrm{Ctr}_k(Qq)} :Qq(\overline{q_{i_1}q_{j_1}} \cdots \overline{q_{i_k}q_{j_k}}):$$

$$= \quad :Qq: + \sum_{k=1}^{\lfloor (n+1)/2 \rfloor} \sum_{(i_1 j_2)\cdots(i_k j_k)}^{\mathrm{Ctr}_k(Qq)} :Qq(\overline{q_{i_1}q_{j_1}} \cdots \overline{q_{i_k}q_{j_k}}):$$

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

Corollary 2.1. *Wick's theorem for operator products.* $:Q::Q': = :QQ': + :\overline{QQ'}:$

Proof: By Wick's theorem $:Q::Q': = :QQ': + :\left(\overline{:Q::Q':}\right):$ and since $:Q:$ and $:Q':$ are in normal order their contractions vanish, leaving $:\left(\overline{:Q::Q':}\right): = :\overline{QQ'}:$.

Corollary 2.2. *Wick's theorem for expectation values.* $\langle \mathrm{vac}|Q|\mathrm{vac}\rangle = :\overline{\overline{Q}}:$

Proof: From Wick's theorem $\langle \mathrm{vac}|Q|\mathrm{vac}\rangle = \langle \mathrm{vac}|:Q:|\mathrm{vac}\rangle + \langle \mathrm{vac}|\overline{Q}:|\mathrm{vac}\rangle$ and any incompletely contractioned have vanishing expectation values by the definition of normal ordering. Therefore, $\langle \mathrm{vac}|:Q:|\mathrm{vac}\rangle = 0$ and $\langle \mathrm{vac}|:\overline{Q}:|\mathrm{vac}\rangle = :\overline{\overline{Q}}:$.

Problem 2.2. Do problem prob 2.1 in reverse: use Wick's theorem to expand $a_p a_q a_s^\dagger a_r^\dagger$ as a linear combination of vac-normal operator strings. Then use cor 2.2 to evaluate $\langle \mathrm{vac}|a_p a_q a_s^\dagger a_r^\dagger|\mathrm{vac}\rangle$.

Proposition 2.1. *Sign rule for completely contracted strings.* *The phase vactor of a completely contracted string is given by $(-)^c$ where c is the number of crossings between contraction lines.*

Proof: Let $\varepsilon_\pi :\overline{q_{\pi(1)}q_{\pi(2)}} \cdots \overline{q_{\pi(n-1)}q_{\pi(n)}}:$ be the disentangled form of a complete contraction of $q_1 \cdots q_n$, where n is an even integer. The phase factor for the contraction, ε_π, is equal to the signature of the disentangling permutation, which is equal to the signature of the inverse permutation π^{-1}, restoring the original ordering of the operators. π^{-1} can be expressed as a series of transpositions between pairs of adjacent operators that are not contracted together. Since every operator has a contraction line overhead, each such transposition changes the number of crossings by exactly ± 1, so $\varepsilon_\pi = (-)^c$ where c is the number of crossings in the original contraction pattern.

Problem 2.3. By expanding $|\Phi\rangle$ as $a_{i_1}^\dagger \cdots a_{i_n}^\dagger |\mathrm{vac}\rangle$, use cor 2.2 to show, using verbal arguments where appropriate, that

$$\langle \Phi|a_p^\dagger a_q|\Phi\rangle = \gamma_{qp} \qquad \langle \Phi|a_p^\dagger a_q^\dagger a_s a_r|\Phi\rangle = \gamma_{rp}\gamma_{sq} - \gamma_{sp}\gamma_{rq} \qquad \gamma_{pq} \equiv \begin{cases} \delta_{pq} & p,q \in \{i_1,\ldots,i_n\} \\ 0 & \text{otherwise.} \end{cases}$$

Use your results to derive the first Slater-Condon rule. The solution of this problem will be substantially simplified in the next section by shifting from vac-normal to Φ-normal ordering.

3. Φ-normal ordering

Definition 3.1. *Hole-particle isomorphism.* The *hole-particle isomorphism* with respect to the reference determinant $|\Phi\rangle = |\underbrace{1\cdots 1}_{n \text{ times}} 0\, 0\cdots\rangle$ is a mapping $F(\mathcal{H}) \to F(\mathcal{H})$ that inverts the bits occupied in Φ:

$$|k_1 \cdots k_n k_{n+1} k_{n+1} \cdots\rangle \mapsto |\overline{k}_1 \cdots \overline{k}_n k_{n+1} k_{n+2} \cdots\rangle \qquad \text{where } \overline{k}_i = 1 - k_i.$$

Physically, this corresponds to shift in perspective from the *particle frame* to a *quasiparticle frame*, where the first n states are viewed as *holes* rather than *particles*. This makes $|\mathrm{vac}\rangle \mapsto |\underbrace{\overline{1}\cdots\overline{1}}_{n \text{ times}} 0\,0\cdots\rangle$ a state of n holes and no particles. $|\Phi\rangle \mapsto |\underbrace{\overline{0}\cdots\overline{0}}_{n \text{ times}} 0\,0\cdots\rangle$ becomes the *quasiparticle vacuum state*, in which all hole and particle states are unoccupied.

Definition 3.2. *Quasiparticle creation and annihilation operators.* If we apply def 1.5 to the new quasiparticle Fock space, we end up with a new system of *quasiparticle-quasihole operators* $\{b_p\} \cup \{b_p^\dagger\}$, related to the old set via

$$a_i \mapsto b_i^\dagger \qquad\qquad a_i^\dagger \mapsto b_i \qquad\qquad a_a \mapsto b_a \qquad\qquad a_a^\dagger \mapsto b_a^\dagger \qquad\qquad (3.1)$$

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

Definition 3.3. Φ-*normal order.* A string $q_1 \cdots q_n$ of particle-hole operators 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 $b_{p_1} \cdots b_{p_m}^\dagger b_{r_1} \cdots b_{r'_m}$ under the hole-particle isomorphism. This guarantees that the quasiparticle vacuum expectation value of the string goes to zero, $\langle \Phi|q_1 \cdots q_n|\Phi\rangle = 0$.

Definition 3.4. Φ-*normal ordering*. The Φ-*normal ordering* of a string $q_1 \cdots q_n$ of particle-hole operators is the mapping $q_1 \cdots q_n \mapsto \text{⦂} q_1 \cdots q_n \text{⦂} \equiv \varepsilon_\pi q_{\pi(1)} \cdots q_{\pi(n)}$ where $\pi \in S_n$ is a permutation that places the string in Φ-normal order.

Definition 3.5. Φ-*normal contraction*. A Φ-*normal contraction* of two particle-hole operators q_1 and q_2 is defined as $\overset{\frown}{q_1 q_2} \equiv q_1 q_2 - \text{⦂} q_1 q_2 \text{⦂}$. This associates a scalar value with every pair in $\{a_p\} \cup \{a_p^\dagger\}$, of which only only those that map to $\overset{\frown}{b_p b_q^\dagger} = b_p^\dagger b_q - \text{⦂} b_p b_q \text{⦂} = [b_p^\dagger, b_q]_+ = \delta_{pq}$, namely $\overset{\frown}{a_a a_b^\dagger} = \delta_{ab}$ and $\overset{\frown}{a_i^\dagger a_j} = \delta_{ij}$, are non-zero.

Definition 3.6. Φ-*normal contractions as pairwise density moments of the quasiparticle vacuum*. Φ-normal contractions can be identified with pairwise moments of the quasiparticle vacuum Φ via $\overset{\frown}{q_1 q_2} = \langle \Phi | q_1 q_2 - \text{⦂} q_1 q_2 \text{⦂} | \Phi \rangle = \langle \Phi | q_1 q_2 | \Phi \rangle$ since $\langle \Phi | \text{⦂} q_1 q_2 \text{⦂} | \Phi \rangle = 0$ by definition. The non-vanishing contractions are elements of the Φ one-hole density matrix, $\overset{\frown}{a_p a_q^\dagger} = \eta_{pq}$, or the Φ one-particle density matrix, $\overset{\frown}{a_p^\dagger a_q} = \gamma_{qp}$. The density matrices η_{pq} and γ_{pq} of a determinant are zero everywhere except the occupied and virtual blocks, respectively, where $\eta_{ab} = \delta_{ab}$ and $\gamma_{ij} = \delta_{ij}$.

Notation 3.1. Φ-*normal-ordered strings with contraction lines*. As in the vac-normal case, we define

$$\text{⦂} q_1 \cdots \overset{\frown}{q_i \cdots q_j} \cdots q_n \text{⦂} \equiv (-)^{j-i-1} \overset{\frown}{q_i q_j} \text{⦂} q_1 \cdots \cancel{q_i} \cdots \cancel{q_j} \cdots q_n \text{⦂} \tag{3.2}$$

where the contraction line now indicates a Φ-normal contraction rather than a vac-normal contraction.

Remark 3.1. *Wick's theorem for Φ-normal ordering*. Since the particle-hole isomorphism maps Φ-normal ordered products with Φ-normal contractions into vac-normal ordered products with vac-normal contractions, Wick's theorem carries over directly as $Q = \text{⦂} Q \text{⦂} + \text{⦂} \overline{Q} \text{⦂}$ where $\text{⦂} \overline{Q} \text{⦂}$ is a sum over all single and multiple Φ-normal contractions. The corollaries $\text{⦂} Q \text{⦂} \text{⦂} Q' \text{⦂} = \text{⦂} QQ' \text{⦂} + \text{⦂} \overline{QQ'} \text{⦂}$ and $\langle \Phi | Q | \Phi \rangle = \text{⦂} \overline{Q} \text{⦂}$ follow.

Problem 3.1. Do prob 2.3 using Wick's theorem for Φ-normal ordering.

Definition 3.7. Φ-*normal component of an operator*. The Φ-*normal component* of a Fock-space operator A is the part of A with a vanishing Φ expectation value, $A_c \equiv A - \langle \Phi | A | \Phi \rangle$. Note that this is generally not the same as the Φ-normal ordering $\text{:} A \text{:}$ of the operator.

Problem 3.2. Using Wick's theorem for Φ-normal ordering, show that vac-normal single and double excitation operators can be expanded in Φ-normal ordered excitation operators as follows.

$$a_p^\dagger a_q = \text{⦂} a_p^\dagger a_q \text{⦂} + \gamma_{qp} \qquad a_p^\dagger a_q^\dagger a_s a_r = \text{⦂} a_p^\dagger a_q^\dagger a_s a_r \text{⦂} - \gamma_{sp} \text{⦂} a_q^\dagger a_r \text{⦂} + \gamma_{rp} \text{⦂} a_q^\dagger a_s \text{⦂} + \gamma_{sq} \text{⦂} a_p^\dagger a_r \text{⦂} - \gamma_{rq} \text{⦂} a_p^\dagger a_s \text{⦂} + \gamma_{rp} \gamma_{sq} - \gamma_{sp} \gamma_{rq}$$

Use these results to derive the following expression for Φ-normal component of H_e.

$$H_c \equiv H_e - \langle \Phi | H_e | \Phi \rangle = \sum_{pq}^\infty f_{pq} \text{⦂} a_p^\dagger a_q \text{⦂} + \tfrac{1}{4} \sum_{pqrs}^\infty \langle pq || rs \rangle \text{⦂} a_p^\dagger a_q^\dagger a_s a_r \text{⦂} \qquad \begin{aligned} f_{pq} &\equiv h_{pq} + \sum_{rs}^\infty \langle pr || qs \rangle \gamma_{sr} \\ \langle pq || rs \rangle &\equiv \langle pq | rs \rangle - \langle pq | sr \rangle \end{aligned} \tag{3.3}$$

4. Kutzelnigg-Mukherjee tensor notation

Notation 4.1. *Kutzelnigg-Mukherjee tensor notation*. In *Kutzelnigg-Mukherjee (KM) tensor ntation*, 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 (def A.1). Furthermore, the Einstein summation convention (nt A.1) is adopted. As usual, indices $i, j, k, l, \ldots$ count over occupied orbitals, indices $a, b, c, d, \ldots$ count over virtual orbitals, and indices $p, q, r, s, \ldots$ count over the full spin-orbital basis. Creation operators are covariant and are therefore denoted $a_p^\dagger \mapsto a^p$, whereas annihilation operators are contravariant and therefore keep their original notation. The one-particle and one-hole density matrices 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. vac-normal ordered and Φ-normal ordered m-fold excitation operators are expressed as tensors in $T_m^m(\mathcal{H})$.

$$a_{q_1 \cdots q_m}^{p_1 \cdots p_m} \equiv a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1} \qquad\qquad \tilde{a}_{q_1 \cdots q_m}^{p_1 \cdots p_m} \equiv \text{⦂} a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1} \text{⦂} \tag{4.1}$$

Remark 4.1. *Permutational symmetries of KM notation excitation operators*. The anticommutation relationships of particle-hole operators impart the following permutational symmetries on KM notation excitation tensors

$$a_{q_1 \cdots q_m}^{p_1 \cdots p_m} = \varepsilon_\pi a_{q_1 \cdots q_m}^{p_{\pi(1)} \cdots p_{\pi(m)}} = \varepsilon_\pi a_{q_{\pi(1)} \cdots q_{\pi(m)}}^{p_1 \cdots p_m} = a_{q_{\pi(1)} \cdots q_{\pi(m)}}^{p_{\pi(1)} \cdots p_{\pi(m)}} \tag{4.2}$$

$$\tilde{a}_{q_1 \cdots q_m}^{p_1 \cdots p_m} = \varepsilon_\pi \tilde{a}_{q_1 \cdots q_m}^{p_{\pi(1)} \cdots p_{\pi(m)}} = \varepsilon_\pi \tilde{a}_{q_{\pi(1)} \cdots q_{\pi(m)}}^{p_1 \cdots p_m} = \tilde{a}_{q_{\pi(1)} \cdots q_{\pi(m)}}^{p_{\pi(1)} \cdots p_{\pi(m)}} \tag{4.3}$$

for all $\pi \in S_n$. Furthermore, the antisymmetry of normal-ordered operator strings permits the following rearrangements.

$$a^{p_1\cdots p_m}_{q_1\cdots q_m} = :a^{p_1}_{q_1} \cdots a^{p_m}_{q_m}: \qquad\qquad :a^{p_1\cdots p_m}_{q_1\cdots q_m} a^{r_1\cdots r_n}_{s_1\cdots s_n}: = :a^{p_1}_{q_1} \cdots a^{p_m}_{q_m} a^{r_1}_{s_1} \cdots a^{r_n}_{s_n}: = a^{p_1\cdots p_m r_1\cdots r_n}_{q_1\cdots q_m s_1\cdots s_n} \qquad (4.4)$$

$$\tilde{a}^{p_1\cdots p_m}_{q_1\cdots q_m} = :a^{p_1}_{q_1} \cdots a^{p_m}_{q_m}: \qquad\qquad :a^{p_1\cdots p_m}_{q_1\cdots q_m} a^{r_1\cdots r_n}_{s_1\cdots s_n}: = :a^{p_1}_{q_1} \cdots a^{p_m}_{q_m} a^{r_1}_{s_1} \cdots a^{r_n}_{s_n}: = \tilde{a}^{p_1\cdots p_m r_1\cdots r_n}_{q_1\cdots q_m s_1\cdots s_n} \qquad (4.5)$$

These symmetries can be used to our advantage in algebraic manipulations of these operators.

Definition 4.1. *m-electron operators in KM notation.* An m-electron operator with non-antisymmetric interaction tensor $v^{q_1\cdots q_m}_{p_1\cdots p_m}$ is expressed in KM notation as

$$V = \tfrac{1}{m!} v^{q_1\cdots q_m}_{p_1\cdots p_m} a^{p_1\cdots p_m}_{q_1\cdots q_m}$$

As shown in prop B.2, any such operator can also be written in terms of an antisymmetrized interaction tensor $\overline{v}^{q_1\cdots q_m}_{p_1\cdots p_m}$ as

$$V = \left(\tfrac{1}{m!}\right)^2 \overline{v}^{q_1\cdots q_m}_{p_1\cdots p_m} a^{p_1\cdots p_m}_{q_1\cdots q_m}$$

where the elements of $\overline{v}$ satisfy $\overline{v}^{q_1\cdots q_m}_{p_1\cdots p_m} = \varepsilon_\pi \overline{v}^{q_1\ \cdots q_m}_{p_{\pi(1)}\cdots p_{\pi(m)}} = \varepsilon_\pi \overline{v}^{q_{\pi(1)}\cdots q_{\pi(m)}}_{p_1\ \cdots p_m}$.

Example 4.1. The vac-normal and Φ-normal components of the electronic Hamiltonian are expressed as

$$H_e = h^q_p a^p_q + \tfrac{1}{2} g^{rs}_{pq} a^{pq}_{rs} \qquad\qquad\qquad H_c = f^q_p \tilde{a}^p_q + \tfrac{1}{4} \overline{g}^{rs}_{pq} \tilde{a}^{pq}_{rs} \qquad (4.6)$$

where $h^q_p \equiv \langle \psi_p(1)|\hat{h}(1)|\psi_q(1)\rangle$, $g^{rs}_{pq} \equiv \langle \psi_p(1)\psi_q(2)|\hat{g}(1,2)|\psi_r(1)\psi_s(2)\rangle$, $f^q_p \equiv h^q_p + \overline{g}^{qs}_{pr}\gamma^r_s$, and $\overline{g}^{rs}_{pq} = g^{rs}_{pq} - g^{sr}_{pq}$.

Definition 4.2. *Bartlett's index permutation operators.* Let $\hat{P}^{(p_1/\cdots/p_m)}_{(q_1/\cdots/q_n)}$ denote an *index permutation operator*, which sums over all permutations of the upper and lower indices $p_1 \cdots p_m$ and $q_1 \cdots q_n$ in a tensor expression, weighted by the permutational signature of each.

$$\hat{P}^{(p_1/\cdots/p_m)}_{(s_1/\cdots/s_n)} t^{p_1\cdots p_m}_{s_1\cdots s_n} \equiv \sum_{\pi\in S_m} \sum_{\sigma\in S_n} \varepsilon_\pi \varepsilon_\sigma t^{p_{\pi(1)}\cdots p_{\pi(m)}}_{s_{\sigma(1)}\cdots s_{\sigma(n)}} \qquad (4.7)$$

Furthermore, let $\hat{P}^{(P_1/\cdots/P_M)}_{(S_1/\cdots/S_N)}$, where $P_i = P_i(1)\cdots P_i(m_i)$ is a block of indices, denote a sum over all permutations except for those that involve transpositions within one of the blocks.

$$\hat{P}^{(P_1/\cdots/P_M)}_{(S_1/\cdots/S_N)} t^{P_1(1)\cdots P_M(m_M)}_{S_1(1)\cdots S_N(n_N)} = \sum_\pi \sum_\sigma \varepsilon_\pi t^{\pi(P_1(1))\cdots \pi(P_M(m_M))}_{\sigma(S_1(1))\cdots \sigma(S_N(n_N))} \qquad \begin{aligned} \pi(P_i(k)) &\begin{cases} = P_i(k) \\ \in \bigcup_{j\neq i} P_j \end{cases} \\[2mm] \sigma(S_i(k)) &\begin{cases} = S_i(k) \\ \in \bigcup_{j\neq i} S_j \end{cases} \end{aligned} \qquad (4.8)$$

That is, the value of $\pi(P_i(k))$ is allowed to be $P_i(k)$ itself or any value in the remaining blocks, P_j with $j \neq i$, but it cannot be any of the other values in P_i, namely $P_i(1), \ldots, P_i(k-1), P_i(k+1), \ldots, P_i(m_i)$. Finally, arguments separated by vertical bars indicate indpendent sets of permutations, $\hat{P}^{(P_1/\cdots/P_M|P'_1/\cdots/P'_{M'})}_{(S_1/\cdots/S_N)} = \hat{P}_{(S_1/\cdots/S_N)} \hat{P}^{(P_1/\cdots/P_M)} \hat{P}^{(P'_1/\cdots/P'_{M'})}$.

Notation 4.2. *Dot notation for contractions.* To allow all of the usual Wick expansions to be expressed, we here augment the traditional KM notation with the following definitions of *particle $\bullet$ contractions* and *hole $\circ$ contractions*.

$$a_{p\bullet} a^{q\bullet} \equiv \overline{a_p a^q} \qquad a^{q\bullet} a_{p\bullet} \equiv -\overline{a_p a^q} \qquad a^{q\circ} a_{p\circ} \equiv \overline{a^q a_p} \qquad a_{p\circ} a^{q\circ} \equiv -\overline{a^q a_p} \qquad (4.9)$$

Note that $a^{p\bullet}_{q\bullet} = -\eta^p_q$ and $a^{p\circ}_{q\circ} = \gamma^p_q$. In vac-normal ordering, the hole contractions vanish and the particle contractions become Kronecker deltas. This notation allows for normal ordered strings with contractions to keep all of the permutational symmetries listed in rmk 4.1.

Problem 4.1. Do problem 3.2 in KM notation by first showing that

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

and then plugging these expressions into H_e to derive H_c.

Example 4.2. *Derivation of CIS equations in KM notation.* A programmable expression for the CI singles Hamiltonian matrix elements, $\langle\Phi_i^a|H_c|\Phi_j^b\rangle$, can be derived in KM notation as follows.

$$\langle\Phi|\tilde{a}_a^i\tilde{a}_q^p\tilde{a}_j^b|\Phi\rangle = {:}a_{a\bullet}^{i\circ}a_{q\bullet\bullet}^{p\bullet}a_{j\circ}^{b\bullet\bullet}{:} + {:}a_{a\bullet}^{i\circ}a_{q\circ}^{p\circ\circ}a_{j\circ\circ}^{b\bullet}{:} = \gamma_j^i\eta_a^p\eta_q^b - \gamma_q^i\gamma_j^p\eta_a^b$$

$$\langle\Phi|\tilde{a}_a^i\tilde{a}_{rs}^{pq}\tilde{a}_j^b|\Phi\rangle = \hat{P}_{(r/s)}^{(p/q)}{:}\tilde{a}_{a\bullet}^{i\circ}\tilde{a}_{r\circ s\bullet\bullet}^{p\bullet q\circ\circ}\tilde{a}_{j\circ\circ}^{b\bullet\bullet}{:} = \hat{P}_{(r/s)}^{(p/q)}\gamma_r^i\eta_a^p\gamma_j^q\eta_s^b$$

$$\implies \langle\Phi_i^a|H_c|\Phi_j^b\rangle = f_p^q\left(\gamma_j^i\eta_a^p\eta_q^b - \gamma_q^i\gamma_j^p\eta_a^b\right) + \tfrac{1}{4}\overline{g}_{pq}^{rs}\left(\hat{P}_{(r/s)}^{(p/q)}\gamma_r^i\eta_a^p\gamma_j^q\eta_s^b\right) = f_a^b\gamma_j^i - f_j^i\eta_a^b + \overline{g}_{aj}^{ib}$$

which simplifies to $\langle\Phi_i^a|H_c|\Phi_j^b\rangle = f_a^b\delta_j^i - f_j^i\delta_a^b + \overline{g}_{aj}^{ib}$. Here, we have used the fact that $\tilde{a}_i^a = a_i^a$ and $\tilde{a}_a^i = a_a^i$.

Problem 4.2. Derive the following results in KM notation using Wick's theorem for expectation values

$$\langle\Phi|a_q^p|\Phi\rangle = \gamma_q^p \qquad \langle\Phi|a_q^pa_i^a|\Phi\rangle = \gamma_i^p\eta_q^a \qquad \langle\Phi|a_q^pa_{ij}^{ab}|\Phi\rangle = 0 \qquad \langle\Phi|a_q^pa_{ijk}^{abc}|\Phi\rangle = 0$$

$$\langle\Phi|a_{rs}^{pq}|\Phi\rangle = \hat{P}_{(r/s)}\gamma_r^p\gamma_s^q \quad \langle\Phi|a_{rs}^{pq}a_i^a|\Phi\rangle = \hat{P}_{(r/s)}^{(p/q)}\gamma_r^p\gamma_i^q\eta_s^a \quad \langle\Phi|a_{rs}^{pq}a_{ij}^{ab}|\Phi\rangle = \hat{P}_{(r/s)}^{(p/q)}\gamma_i^p\gamma_j^q\eta_r^a\eta_s^b \quad \langle\Phi|a_{rs}^{pq}a_{ijk}^{abc}|\Phi\rangle = 0$$

and plug them into $\langle\Phi|H_e|\Phi_{ijk\cdots}^{abc\cdots}\rangle$ to get the Slater-Condon rules.

Example 4.3. *Derivation of CID equations in KM notation.* Projecting the CID Schrödinger equation, $H_c\Psi = E_c\Psi$ with $\Psi = (1 + \tfrac{1}{4}c_{cd}^{kl}\tilde{a}_{kl}^{cd})\Phi$, by Φ and Φ_{ij}^{ab} gives a system of linear equations

$$E_c = \langle\Phi|H_c(1 + \tfrac{1}{4}c_{cd}^{kl}\tilde{a}_{kl}^{cd})|\Phi\rangle \qquad\implies\qquad E_c = \tfrac{1}{4}\langle\Phi|H_c|\Phi_{kl}^{cd}\rangle c_{cd}^{kl}$$

$$E_c c_{ab}^{ij} = \langle\Phi_{ij}^{ab}|H_c(1 + \tfrac{1}{4}c_{cd}^{kl}\tilde{a}_{kl}^{cd})|\Phi\rangle \qquad\implies\qquad E_c c_{ab}^{ij} = \langle\Phi_{ij}^{ab}|H_c|\Phi\rangle + \tfrac{1}{4}\langle\Phi_{ij}^{ab}|H_c|\Phi_{kl}^{cd}\rangle c_{cd}^{kl}$$

which can be simplified into programmable expressions as follows.

$$\begin{aligned}
\langle\Phi|\tilde{a}_{kl}^{pq}\tilde{a}_{kl}^{cd}|\Phi\rangle =&\ \hat{P}_{(r/s)}^{(p/q)}\gamma_k^p\gamma_l^q\eta_r^c\eta_s^d\\
\langle\Phi|\tilde{a}_{ab}^{ij}\tilde{a}_q^p\tilde{a}_{kl}^{cd}|\Phi\rangle =&\ \hat{P}_{(a/b|k/l)}^{(c/d)}{:}\tilde{a}_{a\bullet1b\bullet3}^{i\circ1j\circ2}\tilde{a}_{q\bullet2}^{p\bullet1}\tilde{a}_{k\circ1l\circ2}^{c\bullet2d\bullet3}{:} + \hat{P}_{(k/l)}^{(i/j|c/d)}{:}\tilde{a}_{a\bullet1b\bullet2}^{i\circ1j\circ3}\tilde{a}_{q\circ1}^{p\circ2}\tilde{a}_{k\circ2l\circ3}^{c\bullet1d\bullet2}{:}\\
=&\ \hat{P}_{(a/b|k/l)}^{(c/d)}\eta_a^p\eta_q^c\eta_b^d\gamma_k^i\gamma_l^j - \hat{P}_{(k/l)}^{(i/j|c/d)}\gamma_q^i\gamma_k^p\gamma_l^j\eta_a^c\eta_b^d\\
\langle\Phi|\tilde{a}_{ab}^{ij}\tilde{a}_{rs}^{pq}\tilde{a}_{kl}^{cd}|\Phi\rangle =&\ \hat{P}_{(a/b|k/l)}^{(c/d)}{:}\tilde{a}_{a\bullet1b\bullet2}^{i\circ1j\circ2}\tilde{a}_{r\bullet3s\bullet4}^{p\bullet1q\bullet2}\tilde{a}_{k\circ1l\circ2}^{c\bullet3d\bullet4}{:} + \hat{P}_{(k/l)}^{(i/j|c/d)}{:}\tilde{a}_{a\bullet1b\bullet3}^{i\circ1j\circ2}\tilde{a}_{r\circ1s\circ2}^{p\circ3q\circ4}\tilde{a}_{k\circ3l\circ4}^{c\bullet1d\bullet2}{:} + \hat{P}_{(r/s|k/l|a/b)}^{(p/q|i/j|c/d)}{:}\tilde{a}_{a\bullet1b\bullet3}^{i\circ1j\circ3}\tilde{a}_{r\circ1s\bullet2}^{p\circ2q\bullet1}\tilde{a}_{k\circ2l\circ3}^{c\bullet2d\bullet3}{:}\\
=&\ \hat{P}_{(a/b|k/l)}^{(c/d)}\eta_a^p\eta_b^q\eta_r^c\eta_s^d\gamma_k^i\gamma_l^j + \hat{P}_{(k/l)}^{(i/j|c/d)}\gamma_r^i\gamma_s^j\gamma_k^p\gamma_l^q\eta_a^c\eta_b^d - \hat{P}_{(r/s|k/l|a/b)}^{(p/q|i/j|c/d)}\gamma_r^i\gamma_k^p\gamma_l^j\eta_a^q\eta_s^c\eta_b^d
\end{aligned}$$

$$\implies \qquad E_c = \tfrac{1}{4}\overline{g}_{kl}^{cd}c_{cd}^{kl} \qquad E_c c_{ab}^{ij} = \overline{g}_{ab}^{ij} + \hat{P}_{(a/b)}f_a^c c_{cb}^{ij} - \hat{P}^{(i/j)}f_k^i c_{ab}^{kj} + \tfrac{1}{2}\overline{g}_{ab}^{cd}c_{cd}^{ij} + \tfrac{1}{2}\overline{g}_{kl}^{ij}c_{ab}^{kl} + \hat{P}_{(a/b)}^{(i/j)}\overline{g}_{ak}^{ic}c_{bc}^{jk}$$

Problem 4.3. Derive the Φ-normal Wick expansion for triple excitations

$$a_{stu}^{pqr} = \tilde{a}_{stu}^{pqrs} + \hat{P}_{(s/tu)}^{(p/qr)}\gamma_s^p\tilde{a}_{tu}^{qr} + \hat{P}_{(s/t/u)}^{(pq/r)}\gamma_s^p\gamma_t^q\tilde{a}_u^r + \hat{P}_{(s/t/u)}\gamma_s^p\gamma_t^q\gamma_u^r$$

where $\hat{P}_{(p/q/r)}t_{pqr} = t_{pqr} - t_{prq} - t_{qpr} + t_{qrp} + t_{rpq} - t_{rqp}$ and $\hat{P}_{(p/qr)}t_{pqr} = t_{pqr} - t_{qpr} - t_{rqp}$.

A. Tensors

Definition A.1. *Covariance, contravariance, invariance.* Let ϕ be an arbitrary linear function of a vector space V and consider a change of basis $\{e_1, \cdots, e_n\} \to \{\tilde{e}_1, \cdots, \tilde{e}_n\}$ defined by $\tilde{e}_j = \sum_i e_i [\mathbf{T}]_{ij}$ where $\mathbf{T}$ is an invertible matrix. If ϕ obeys the same transformation law as the basis elements, it is a *covariant* quantity. If it obeys the opposite transformation law, it is a *contravariant* quatntity.

$$\phi(\tilde{e}_j) = \sum_i \phi(e_i) [\mathbf{T}]_{ij} \qquad (covariant) \qquad \phi(\tilde{e}_i) = \sum_j [\mathbf{T}^{-1}]_{ij} \phi(e_j) \qquad (contravariant) \qquad (A.1)$$

Covariant quantities are typically denoted with subscript indices, $\phi_i = \phi(e_i)$, whereas *contravariant* quantities are denoted with superscript indices, $\phi^i = \phi(e_i)$. Abstract quantities such as vectors and operators are called *invariant*, since they do not depend on the choice of basis.

Example A.1. *Vector coordinates are contravariant.* Let $\{v_i\}$ be the coordinates of a vector v in the basis $\{e_i\}$, and let $\{\tilde{v}_j\}$ be its coordinates in $\{\tilde{e}_j = \sum_i e_i [\mathbf{T}]_{ij}\}$. Then the invariance of v implies that the coordinates are contravariant:

$$\sum_i e_i v_i = v = \sum_j \tilde{e}_j \tilde{v}_j = \sum_i e_i \sum_j [\mathbf{T}]_{ij} \tilde{v}_j \implies v_i = \sum_j [\mathbf{T}]_{ij} \tilde{v}_j \implies \tilde{v}_j = \sum_i [\mathbf{T}^{-1}]_{ji} v_i$$

Therefore, vector coordinates should be written with superscript indices $v_i \mapsto v^i$.

Definition A.2. *Linear functional.* A *linear functional* $f : V \to \mathbb{C}$ is a scalar-valued function on V that satisfies $f(v+w) = f(v) + f(w)$ and $f(cv) = cf(v)$ for all $c \in \mathbb{C}$ and all $v, w \in V$. The *null functional* is given by $f_0(v) = 0 \; \forall v \in V$.

Definition A.3. *Dual space V^*.* The *dual space* of V, denoted V^*, is the space of linear functionals on V, which itself forms a vector space with respect to vector addition $(f + g) \in V^*$ and scalar multiplication $(cf) \in V^*$ defined by

$$(f + g)(v) \equiv f(v) + g(v) \qquad\qquad (cf)(v) \equiv cf(v) \qquad\qquad (A.2)$$

for all $f, g \in V^*$, $v \in V$, and $c \in \mathbb{C}$. Its dimension is $\dim V^* = \dim V$, which follows from prop A.1.

Proposition A.1. *The canonical dual basis.* *If $\{e_1, \cdots, e_n\}$ is a basis for V then $\{e^1, \cdots, e^n\} \subset V^*$, defined by $e^i(e_j) = \delta^i_j$, is a basis for V^*. This "canonical dual basis" transforms contravariantly relative to $\{e_1, \cdots, e_n\}$.*
    Proof: First, note that $e^j(v) = e^j(\sum_i e_i v^i) = \sum_i e^j(e_i) v^i = v^j$ for any $v \in V$. Therefore, $f(v) = f(\sum_i e_i v^i) = \sum_i f(e_i) v^i = \sum_i f(e_i) e^i(v)$ holds for all $f \in V^*$ and all $v \in V$, which implies that $f = \sum_i f(e_i) e^i$. This shows that $\text{span}\{e^1, \cdots, e^n\} = V^*$. Second, assume there exist $c_j \in \mathbb{C}$ such that $\sum_j c_j e^j = f_0$, where f_0 is the null functional. Then $0 = f_0(e_i) = \sum_j c_j e^j(e_i) = c_i$ and all of the coefficients must be zero, showing that $\{e^1, \cdots, e^n\}$ is linearly independent. Since both sets have n elements, $\dim V = \dim V^*$. Since $v^j = e^j(v)$, the dual basis is contravariant.

Remark A.1. If $\langle \cdot | \cdot \rangle$ is an inner product on V and $\mathbf{S}$ is the matrix of overlaps, $\langle e_i | e_j \rangle = [\mathbf{S}]_{ij}$, then the canonical dual basis is given by $e^i(\cdot) = \sum_j [\mathbf{S}^{-1}]_{ij} \langle e_j | \cdot \rangle$, which simplifies to $e^i(\cdot) = \langle e_i | \cdot \rangle$ when $\{e_1, \cdots, e_n\}$ is orthonormal.

Definition A.4. *Linear operator.* A *linear operator* $\hat{T} : V \to V$ is a vector-valued function on V that satisfies $\hat{T}(v + w) = \hat{T}v + \hat{T}w$ and $\hat{T}(cv) = c\hat{T}v$. The *identity operator* is given by $\hat{1}v = v$ and the *null operator* is given by $\hat{0}v = v$.

Proposition A.2. *Resolution of the identity.* *Given a basis $\{e_i\}$, the identity operator can be expressed as $\hat{1} = \sum_i e_i e^i$.*
    Proof: $\hat{1}(v) = v = \sum_i e_i v^i = \sum_i e_i e^i(v)$ holds for all $v \in V$ (see prop A.1), so $\hat{1} = \sum_i e_i e^i$.

Remark A.2. Using prop A.2, we can identify the matrix of a linear operator, $\hat{T}e_j = \sum_i e_i [\mathbf{T}]_{ij}$, with $[\mathbf{T}]_{ij} = e^i(\hat{T}e_j)$. Therefore, the row index of $\mathbf{T}$ should be written as a superscript index, $[\mathbf{T}]_{ij} \mapsto [\mathbf{T}]^i_j$. Using two resolutions of the identity, $\hat{T}$ can be expressed as $\hat{T} = \sum_{ij} [\mathbf{T}]^i_j e_i e^j$, which identifies $\mathbf{T}$ as its coordinates in $V \times V^* = \text{span}\{e_i e^j\}$.

Remark A.3. The formula for matrix multiplication also follows from prop A.2: the matrix of $\hat{T}\hat{T}'$ is $e^i(\hat{T}\hat{T}'e_j) = \sum_k e^i(\hat{T}e_k) e^k(\hat{T}'e_j) = \sum_k [\mathbf{T}]^i_k [\mathbf{T}']^k_j$.

Definition A.5. *Direct sum $V \oplus V'$.* A *direct sum* of vector spaces V and V' is $V \oplus V' \equiv \{v \oplus v' \,|\, v \in V, v' \in V'\}$, a new vector space with vector addition and scalar multiplication defined by

$$v_1 \oplus v'_1 + v_2 \oplus v'_2 = (v_1 + v_2) \oplus (v'_1 + v'_2) \qquad\qquad c(v \oplus v') = cv \oplus cv' . \qquad (A.3)$$

If $\{e_i\}$ and $\{e'_{i'}\}$ are bases for V and V' then $\{e_i \oplus 0'\} \cup \{0 \oplus e'_{i'}\}$ is a basis for $V \oplus V'$, which has dimension $\dim V + \dim V'$.

Definition A.6. Tensor product $V \otimes V'$. A *tensor product* of vector spaces V and V' is $V \otimes V' \equiv \{\sum v \otimes v' \mid v \in V, v' \in V'\}$, a new vector space with vector addition and scalar multiplication defined by

$$v_1 \otimes v' + v_2 \otimes v' = (v_1 + v_2) \otimes v' \qquad v \otimes v'_1 + v \otimes v'_2 = v \otimes (v'_1 + v'_2) \qquad c(v \otimes v') = (cv) \otimes v' = v \otimes (cv') \quad \text{(A.4)}$$

If $\{e_i\}$ and $\{e'_{i'}\}$ are bases for V and V' then $\{e_i \otimes e'_{i'}\}$ is a basis for $V \otimes V'$, which has dimension $\dim V \cdot \dim V'$.

Remark A.4. Since the sum $S + S'$ of two mutually orthogonal subspaces $S, S \subseteq V$ is isomorphic to their direct sum, $S \oplus S'$ and $S + S'$ are used interchangeably in this context. The reverse is also true. The direct sum of two distinct vector spaces $V \oplus V'$ contains copies of V and V' as mutually orthogonal subspaces, namely $V \simeq V \oplus 0'$ and $V' \simeq 0 \oplus V'$.

Definition A.7. Direct sums and tensor products of inner product spaces. If V and V' are inner product spaces, then $V \oplus V'$ and $V \otimes V'$ are also inner product spaces with respect to the following inner products.

$$\langle v \oplus v' | w \oplus w' \rangle_{V \oplus V'} \equiv \langle v | w \rangle_V + \langle v' | w' \rangle_{V'} \qquad\qquad \langle v \otimes v' | w \otimes w' \rangle_{V \otimes V'} \equiv \langle v | w \rangle_V \cdot \langle v' | w' \rangle_{V'} \qquad \text{(A.5)}$$

Definition A.8. Tensor. A *tensor* is a vector in a tensor product space. An nth *order tensor* lives in a product of n vector spaces, $V_1 \otimes \cdots \otimes V_n$. A *type-(m,n) tensor on V* lives in $\underbrace{V \otimes \cdots \otimes V}_{m \text{ times}} \otimes \underbrace{V^* \otimes \cdots \otimes V^*}_{n \text{ times}}$, denoted $T^m_n(V)$.

Example A.2. $T^0_0(V)$ is the scalar field $\mathbb{C}$, $T^1_0(V)$ is the vector space itself, $T^0_1(V)$ is the dual space V^*, and $T^1_1(V)$ is (up to isomorphism) the space of linear operators $V \otimes V^* \simeq V \times V^*$.

Remark A.5. A member t of $T^m_n(V)$ can be expanded in the basis $\{e_1, \cdots, e_n\}$ as follows.

$$t = \sum_{\substack{i_1 \cdots i_m \\ j_1 \cdots j_n}} t^{i_1 \cdots i_m}_{j_1 \cdots j_n} e_{i_1} \otimes \cdots \otimes e_{i_m} \otimes e^{j_1} \otimes \cdots \otimes e^{j_n} \qquad \text{(A.6)}$$

Its coordinate array $\mathbf{t} = [t^{i_1 \cdots i_m}_{j_1 \cdots j_n}]$ is indexed by m contravariant indices and n covariant indices.

Remark A.6. Just as people often use the term "vector" to refer to the basis-dependent coordinate array v^i rather than v itself, more often than not the word "tensor" refers to the coordinate array $t^{i_1 \cdots i_m}_{j_1 \cdots j_n}$ rather than the abstract quantity t.

Definition A.9. Tensor product $t \otimes t'$. The *tensor product* of $t \in T^m_n(V)$ and $t' \in T^{m'}_{n'}(V)$ is $t \otimes t' \in T^{m+m'}_{n+n'}(V)$ with coordinate array $[\mathbf{t} \otimes \mathbf{t}']^{i_1 \cdots i_{m+m'}}_{j_1 \cdots j_{n+n'}} = t^{i_1 \cdots i_m}_{j_1 \cdots j_n} t^{i_{m+1} \cdots i_{m+m'}}_{j_{n+1} \cdots j_{n+n'}}$. This generalizes the *matrix Kronecker product*.

Definition A.10. Tensor contraction. A (p,q) *tensor contraction* is a map $\text{tr}_{p,q} : T^m_n(V) \to T^{m-1}_{n-1}(V)$ given by tracing the pth element in V with the qth element in V^*:

$$\text{tr}_{p,q}\left(e_{i_1} \otimes \cdots \otimes e_{i_p} \otimes \cdots \otimes e^{j_q} \otimes \cdots \otimes e^{j_n}\right) = \delta^{j_q}_{i_p} e_{i_1} \otimes \cdots \otimes \cancel{e_{i_p}} \otimes \cdots \otimes \cancel{e^{j_q}} \otimes \cdots \otimes e^{j_n} \qquad \text{(A.7)}$$

The coordinate array of $\text{tr}_{p,q}(t)$ is $[\text{tr}_{p,q}(\mathbf{t})]^{i_1 \cdots \cancel{i_p} \cdots i_m}_{j_1 \cdots \cancel{j_q} \cdots j_m} = \sum_{i_p, j_q} \delta^{j_q}_{i_p} t^{i_1 \cdots i_m}_{j_1 \cdots j_m}$, generalizing the *matrix trace*, $\text{tr}(M) = \sum_i M^i_i$.

Definition A.11. Cross-contraction. A *cross-contraction* traces a lower index on one tensor with an upper index on another, $\text{tr}_{p,q'} : T^m_n(V) \otimes T^{m'}_{n'}(V) \to T^m_{n-1}(V) \otimes T^{m'-1}_{n'}(V)$, generalizing the *matrix product* $\text{tr}_{1,1'}(M \otimes M') = \sum_k M^i_k M^k_j$.

Notation A.1. Einstein summation convention. In the *Einstein summation convention* any index which appears twice in a product, once as a covariant index and once as a contravariant one, is implicitly summed over: $\sum_i a_i b^i \mapsto a_i b^i$. For most purposes, this rule suffices to dispense with summation symbols altogether. The basis expansion of a vector now takes the form $v = e_i v^i$, that of a tensor takes the form $t = t^{i_1 \cdots i_m}_{j_1 \cdots j_n} e_{i_1} \otimes \cdots \otimes e_{i_m} \otimes e^{j_1} \otimes \cdots \otimes e^{j_n}$, and resolution of the identity can be written as $\hat{1} = e_i e^i$. The choice of symbol for a *contracted index* is is arbitrary, whereas each *free (uncontracted) index* symbol must appear once in every term on the right- and left-hand sides of an equation, always with the same co- or contra-variance.

Example A.3. In Einstein notation, the matrix expression $\mathbf{C} = \mathbf{AB}$ is written as $C^i_j = A^i_k B^k_j$.

Example A.4. The expression $a^{kl}_{ij} = \frac{1}{2} b^{vx}_{ij} c^{kl}_{vx} + \frac{1}{6} d^{xyz}_{ijv} e^{klv}_{xyz}$ is a balanced equation with free indices $^{kl}_{ij}$. Each term is an element of $T^2_2(V)$, so the addition ($+$) and assignment ($=$) operations are well-defined.

B. Parenthetical results

Proposition B.1. *Pull-through relation.* *For any non-commuting $x_1, \ldots, x_n$, and y for which addition, subtraction and multiplication are defined, $x_1 \cdots x_n y = (\mp)^n \, y x_1 \cdots x_n + \sum_{k=1}^n (\mp)^{n-k} x_1 \cdots [x_k, y]_\pm \cdots x_n$, where $[x, y]_\pm \equiv xy \pm yx$.*
   Proof: The $n = 1$ case folows from the definition of the commutator brackets: $xy = \mp yx + [x, y]_\pm$. Now, assume it holds for n and consider the $n + 1$ case. 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

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

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

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

Proposition B.2. *Expressing m-electron operators in terms of ordinary and antisymmetrized integrals.* *A first-quantized m-electron operator $\hat{V} = \sum_{i_1 < \cdots < i_m} \hat{v}(i_1 \cdots i_m)$ can be expressed in two equivalent second-quantized forms*

$$V = \frac{1}{m!} \sum_{\substack{p_1 \cdots p_m \\ q_1 \cdots q_m}} \langle p_1 \cdots p_m | \hat{v} | q_1 \cdots q_m \rangle a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1} = \left(\frac{1}{m!} \right)^2 \sum_{\substack{p_1 \cdots p_m \\ q_1 \cdots q_m}} \langle p_1 \cdots p_m | \hat{v} | q_{[1} \cdots q_{m]} \rangle a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1}$$

where $\langle p_1 \cdots p_m | \hat{v} | q_{[1} \cdots q_{m]} \rangle \equiv \sum \varepsilon_\pi \langle p_1 \cdots p_m | \hat{v} | q_{\pi(1)} \cdots q_{\pi(m)} \rangle$ are antisymmetrized m-electron integrals and the original m-electron integrals are given by $\langle p_1 \cdots p_m | \hat{v} | q_1 \cdots q_m \rangle \equiv \int d(1 \cdots m) \psi_{p_1}^*(1) \cdots \psi_{p_m}^*(m) \hat{v}(1 \cdots m) \psi_{q_1}(1) \cdots \psi_{q_m}(m)$.
   Proof: It follows from rmk 1.1 that any function Ψ in Fock space can be decomposed as

$$\Psi(1, \cdots, n) = \frac{1}{\sqrt{m!}} \sum_{p_1 \cdots p_m} \psi_{p_1}(1) \cdots \psi_{p_m}(m) (\hat{a}_{p_m} \cdots \hat{a}_{p_1} \Psi)(m, \cdots, n)$$

and therefore the following holds for all $\Psi, \Psi' \in F(\mathcal{H})$

$$\langle \Psi | \hat{V} \Psi' \rangle = \sum_{i_1 < \cdots < i_m}^n \langle \Psi | \hat{v}(i_1 \cdots i_m) \Psi' \rangle = \frac{n!}{m!(n-m)!} \langle \Psi | \hat{v}(1 \cdots m) \Psi' \rangle$$

$$= \frac{1}{m!} \sum_{\substack{p_1 \cdots p_m \\ q_1 \cdots q_m}}^\infty \langle p_1 \cdots p_m | \hat{v} | q_1 \cdots q_m \rangle \langle \hat{a}_{p_m} \cdots \hat{a}_{p_1} \Psi | \hat{a}_{q_m} \cdots \hat{a}_{q_1} \Psi' \rangle$$

which gives the first part of the proposition.

$$V = \frac{1}{m!} \sum_{\substack{p_1 \cdots p_m \\ q_1 \cdots q_m}} \langle p_1 \cdots p_m | \hat{v} | q_1 \cdots q_m \rangle a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1}$$

The antisymmetrized form can then be derived by the following rearrangement

$$V = \frac{1}{m!} \sum_{\substack{p_1 \cdots p_m \\ q_1 \cdots q_m}} \langle p_1 \cdots p_m | \hat{v} | q_1 \cdots q_m \rangle \, a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1}$$

$$= \left(\frac{1}{m!} \right)^2 \sum_{\substack{p_1 \cdots p_m \\ q_1 \cdots q_m}} \sum_{\pi \in S_m} \langle p_1 \cdots p_m | \hat{v} | q_{\pi(1)} \cdots q_{\pi(m)} \rangle \, a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_{\pi(m)}} \cdots a_{q_{\pi(1)}}$$

$$= \left(\frac{1}{m!} \right)^2 \sum_{\substack{p_1 \cdots p_m \\ q_1 \cdots q_m}} \sum_{\pi \in S_m} \varepsilon_\pi \langle p_1 \cdots p_m | \hat{v} | q_{\pi(1)} \cdots q_{\pi(m)} \rangle \, a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{q_m} \cdots a_{q_1}$$

where the first step follows from simply relabeling the dummy indices of summation $q_1 \cdots q_m$ in $m!$ different ways and the second step follows from the fact that annihilation operators anticommute with other annihilation operators.