WICK'S THEOREM

Lemma 1:

$$n[M_1 \ldots M_m]\, M_{m+1}$$
$$= n[M_1 \ldots M_m M_{m+1}]$$
$$+ \sum_{i=1}^{m} n[M_1 \ldots M_i \ldots M_m M_{m+1}]$$

Proof (sketch):

case A (easy)

$$M_{m+1} = X_r^+ \text{ or } X_r$$

case B (difficult)

$$n[M_1 \ldots M_m] X_r^+$$

$$= n[M_1 \ldots M_m X_r^+] + \sum_{i=1}^{m} n[M_1 \ldots \hat{M_i} \ldots M_m X_r^+]$$

B1: all $M_1, \ldots, M_m$ are annihilators

|| hard

B2: there are some creators among $M_1, \ldots, M_m$

easier

$$\Downarrow$$

$$n[X_{p_1} \cdots X_{p_m}]\, X_r^{+}$$

<u>MUST</u> PROVE

$$n[X_{p_1} \cdots X_{p_m} X_r^{+}] + \sum_{i=1}^{m} n[X_{p_1} \cdots X_{p_i} \cdots X_{p_m} X_r^{+}]$$

proof by induction (videos 6,7)

B2 (proof by reduction to B1, video 7)

$$(-1)^R \left(X^\dagger_{p_{R_1}} \cdots X^\dagger_{p_{R_k}} X_{p_{R_{k+1}}} \cdots X_{p_{R_m}}\right) X^\dagger_r$$

$$= (-1)^R n\left[X^\dagger_{p_{R_1}} \cdots X^\dagger_{p_{R_k}} X_{p_{R_{k+1}}} \cdots X_{p_{R_m}} X^\dagger_r\right]$$

$$\cancel{+ (-1)^R \sum_{i=1}^{k} n\left[X^\dagger_{p_{R_1}} \cdots X^\dagger_{p_{R_i}} \cdots X^\dagger_{p_{R_k}} X_{p_{R_{k+1}}} \cdots X_{p_{R_m}} X^\dagger_r\right]} \; 0$$

$$+ (-1)^R \sum_{i=k+1}^{m} n\left[X^\dagger_{p_{R_1}} \cdots X^\dagger_{p_{R_k}} X_{p_{R_{k+1}}} \cdots X_{p_{R_i}} \cdots X_{p_{R_m}} X^\dagger_r\right]$$

$$\left(X^{+}_{P_{R_1}} \cdots X^{+}_{P_{R_k}}\right) n \left[X_{P_{R_{k+1}}} \cdots X_{P_{R_m}}\right] X^{+}_{r}$$

$$= \left(X^{+}_{P_{R_1}} \cdots X^{+}_{P_{R_k}}\right) n \left[X_{P_{R_{k+1}}} \cdots X_{P_{R_m}} X^{+}_{r}\right]$$

$$+ \left(X^{+}_{P_{R_1}} \cdots X^{+}_{P_{R_k}}\right) \sum_{i=k+1}^{m} n \left[X_{P_{R_{k+1}}} \cdots X_{P_{R_i}} \cdots X_{P_{R_m}} X^{+}_{r}\right]$$

$\longrightarrow$ case B1

$\therefore$

Lemma 2:

$$n[M_1 \ldots M_i \ldots M_m]\, M_{m+1}$$

$i \in C$ (indices of operators involved in contractions on the lhs)

$$= n[M_1 \ldots M_i \ldots M_m\, M_{m+1}]$$

same as on the lhs

$$+ \sum_{j=1,\, j \notin C}^{m} n[M_1 \ldots M_i \ldots M_j \ldots M_m\, M_{m+1}]$$

Proof by reduction to Lemma 1.

PROOF OF WICK's THEOREM (WT)

(by induction)

m operators: $M_1, \dots, M_m$

Start with $m=1$:

$$M_1 = n[M_1]$$

$m=2$:

$$M_1 M_2 = n[M_1 M_2] + n[\underbrace{M_1 M_2}]$$

$$= n[M_1 M_2] + \underbrace{M_1 M_2}$$

(definition of contraction)

Induction step

Assume that WT holds for $m = l$ and prove that it remains true for $m = l+1$ using Lemmas 1 and 2.

lemma 1 (1)

$$M_1 \dots M_l M_{l+1} = n[M_1 \dots M_l] M_{l+1}$$

lemma 2 (2)

$$+ \sum_{1 \le i < j \le l} n[M_1 \dots M_{\bar{i}} \dots M_{\bar{j}} \dots M_l] M_{l+1}$$

lemma 2 (3)

$$+ \sum_{\substack{i_1 < j_1 \\ i_2 < j_2 \\ i_1 < i_2,\ j_1 \neq j_2 \\ \le l}} n[M_1 \dots M_{\bar{i}_1} \dots M_{\bar{j}_1} \dots M_{\bar{i}_2} \dots M_{\bar{j}_2} \dots M_l] M_{l+1}$$

odd l

$$+ \dots + \left[\sum_{\dots k = 1, l} n[M_1 \dots M_{k-1} M_k M_{k+1} \dots M_l] M_{l+1} \quad \dots \right.$$

lemma 2

(OR)

$$(+)\sum_{\text{fully contracted (f.c.)}} n\left[\left[M_{i}\ldots M_{i}\ldots M_{j}\ldots M_{\ell}\right] M_{\ell+1}\right]$$

even ℓ

$$= n[M_1 \ldots M_\ell M_{\ell+1}] \quad ①$$

$$+ \sum_{k=1}^{L} n[M_1 \ldots M_k \ldots M_\ell M_{\ell+1}] \quad ①$$

$$+ \sum_{i_1 < j_1 \, (\leq \ell)} n[M_1 \ldots M_{i_1} \ldots M_{j_1} \ldots M_\ell M_{\ell+1}] \quad ②$$

$$+ \sum_{\substack{i_1 < j_1 \, (\leq \ell) \\ k = 1, \ldots, \ell,\ k \neq i_1, j_1}} n[M_1 \ldots M_{i_1} \ldots M_{j_1} \ldots M_k \ldots M_\ell M_{\ell+1}] \quad ②$$

3

$$+\sum_{\substack{i_1<j_1\\ i_2<j_2\\ i_1<i_2,\, j_1\neq j_2}} n[M_1\dots \underbrace{M_{i_1}\dots M_{j_1}}\dots \underbrace{M_{i_2}\dots M_{j_2}}\dots M_\ell M_{\ell+1}]$$

$<\ell$

3

$$+\sum_{\substack{i_1<j_1\\ i_2<j_2\\ i_1<i_2,\, j_1\neq j_2\\ k\neq i_1, j_1, i_2, j_2}} n[M_1\dots \underbrace{M_{i_1}\dots M_{j_1}}\dots \underbrace{M_k\dots \underbrace{M_{i_2}\dots M_{j_2}}\dots M_\ell M_{\ell+1}}]$$

$<\ell$

$+\dots$

$$= n[M_1 \cdots M_\ell M_{\ell+1}]$$

$$+ \sum_{1 \le i_1 < j_1 \le \ell+1} n[M_1 \cdots M_{i_1} \cdots M_{j_1} \cdots M_\ell M_{\ell+1}]$$

$$+ \sum_{\substack{i_1 < j_1 \\ i_2 < j_2 \le \ell+1 \\ i_1 < i_2,\ j_1 \neq j_2}} n[M_1 \cdots M_{i_1} \cdots M_{j_1} \cdots M_{i_2} \cdots M_{j_2} \cdots M_\ell M_{\ell+1}]$$

$$+ \cdots$$

$$\therefore$$

GENERALIZED WICK'S THEOREM (GWT)

$$M_1 \ldots M_{k_{\mu-1}} \, \underbrace{n[M_{k_{\mu-1}+1} \ldots M_{k_\mu}]}_{} \, M_{k_\mu+1} \ldots M_m$$

$$= n[M_1 \ldots M_m]$$

$$+ \sum_{i<j}{}' \, n[M_1 \ldots \underbrace{M_i \ldots M_j} \ldots M_m]$$

$$+ \sum_{\substack{i_1<i_2, \; i_1<j_1, \; i_2<j_2 \\ j_1 \neq j_2}}{}' \, n[M_1 \ldots \underbrace{M_{i_1} \ldots M_{j_1}} \ldots \underbrace{M_{i_2} \ldots M_{j_2}} \ldots M_m]$$

$+ \ldots$

$\sum{}' \rightarrow$ exclude contractions involving operators originating from the same normal product

Proof by reduction to WT and recognition that

$\underbrace{X^\dagger X}$, $\underbrace{X X^\dagger}$, and $\underbrace{X X}$

are all zero.

Example:

$$n[M_1 M_2]\, n[M_3 M_4]$$

$$= n[M_1 M_2 M_3 M_4]$$

$$+ n[M_1 M_2 M_3 M_4]$$

$$+ n[M_1 M_2 M_3 M_4]$$

$$+ n[M_1 M_2 M_3 M_4]$$

$$+ n[M_1 M_2 M_3 M_4]$$

$$+ \quad n[M_1 M_2 M_3 M_4]$$

$$+ \quad n[M_1 M_2 M_3 M_4]$$

Rules 1–4:

$$\langle 0 | \, n[M_1 \ldots M_m] \, | 0 \rangle$$

← without or with contractions

$$n[M_1 \ldots M_m] \, | 0 \rangle$$

Rule 5:

$$\langle 0| M_1 \ldots M_{2m+1} |0\rangle = 0$$

(use WT and rules 2 and 4')

Rule 6:

$$\langle 0| M_1 \ldots M_{2m} |0\rangle$$

$$= \sum_{f.c.} \langle 0| n[M_1 \ldots M_{2m}] |0\rangle$$

$$= \sum_{f.c.} \overset{\pm}{(-1)^R}\ \overset{\text{0 or 1}}{\underbrace{M_{i_1} M_{j_1}}} \ldots \overset{\text{0 or 1}}{\underbrace{M_{i_m} M_{j_m}}}$$

$$R = \begin{pmatrix} 1 & 2 & \cdots & (2m-1) & (2m) \\ i_1 & j_1 & \cdots & i_m & j_m \end{pmatrix}$$

(use WT and rules 2 and 4)

Rule 7:

$$M_1 \cdots M_m |0\rangle$$

$$= \sum_{\text{a.f.c.}} n[M_1 \cdots M_m] |0\rangle$$

(annihilators fully contracted)

$$= \sum_{\text{a.f.c.}} (-1)^R \overbrace{\left(\prod_{i_k j_k \in C} M_{i_k} M_{j_k} \right)}^{\text{coefficients}} \underbrace{\prod_{r \notin C} X_r^\dagger |0\rangle}_{\text{Slater determinants}}$$

indices of contracted operators

(use WT and rules 1 and 3)

Example $n[X_q^\dagger X_r]$

$$\langle 0| X_p \overbrace{X_q^\dagger X_r} X_s^\dagger |0\rangle$$

$$\overset{\text{rule 6}}{\underset{\text{f.c.}}{=}} \langle 0| n[X_p X_q^\dagger X_r X_s^\dagger] |0\rangle$$

$$+ \cancel{\langle 0| n[X_p X_q^\dagger X_r X_s^\dagger] |0\rangle} \to 0$$

$$+ \cancel{\langle 0| n[X_p X_q^\dagger X_r X_s^\dagger] |0\rangle} \to 0$$

$$= \delta_{pq}\, \delta_{rs} \quad \checkmark$$

Verification:

$$X_p X_q^\dagger X_r X_s^\dagger$$

$$\overset{WT}{=} -X_q^\dagger X_s^\dagger X_p X_r$$

$$- \delta_{pq} X_s^\dagger X_r + \delta_{ps} X_q^\dagger X_r$$

$$- \delta_{rs} X_q^\dagger X_p + \delta_{pq}\delta_{rs}$$

$$\langle 0| X_p X_q^\dagger X_r X_s^\dagger |0\rangle$$

$$= \delta_{pq}\delta_{rs}$$

$$S = \langle \{p_1 \ldots p_N\} | \{q_1, \ldots, q_N\} \rangle$$

$$\Updownarrow$$

$$\langle \Phi_{p_1 \ldots p_N} | \Phi_{q_1 \ldots q_N} \rangle$$

$$|\Phi_{p_1 \ldots p_N}\rangle = X^{\dagger}_{p_1} \ldots X^{\dagger}_{p_N} |0\rangle$$

$$|\Phi_{q_1 \ldots q_N}\rangle = X^{\dagger}_{q_1} \ldots X^{\dagger}_{q_N} |0\rangle$$

$$S = \langle 0 | \underbrace{X_{p_N} \ldots X_{p_1}}_{n[X_{p_N} \ldots X_{p_1}]} \underbrace{X^{\dagger}_{q_1} \ldots X^{\dagger}_{q_N}}_{n[X^{\dagger}_{q_1} \ldots X^{\dagger}_{q_N}]} |0\rangle$$

rule6

$$= \sum \langle 0 | n[X_{p_N} \ldots X_{p_1} X^\dagger_{q_1} \ldots X^\dagger_{q_N}] | 0 \rangle$$

f.e.

$$= \sum_{R \in S_N} (-1)^R$$

$$\times \langle 0 | X_{p_N} \ldots X_{p_2} X_{p_1} X^\dagger_{q_{R_1}} X^\dagger_{q_{R_2}} \ldots X^\dagger_{q_{R_N}} | 0 \rangle$$

$$= \sum_{R \in S_N} (-1)^R \overset{\delta_{p_1 q_{R_1}}}{\langle p_1 | q_{R_1} \rangle} \overset{\delta_{p_2 q_{R_2}}}{\langle p_2 | q_{R_2} \rangle}$$

$$\times \ldots \times \underset{\delta_{p_N q_{R_N}}}{\langle p_N | q_{R_N} \rangle}$$

$$= \begin{vmatrix} \langle p_1|q_1\rangle & \cdots & \langle p_1|q_N\rangle \\ & \cdots & \\ \langle p_N|q_1\rangle & \cdots & \langle p_N|q_N\rangle \end{vmatrix}$$

If $p_1 < p_2 < \cdots < p_N$,
$q_1 < q_2 < \cdots < q_N$,

$$\langle \Phi_{p_1 \cdots p_N} | \Phi_{q_1 \cdots q_N} \rangle$$
$$= \delta_{p_1 q_1} \cdots \delta_{p_N q_N}$$

MATRIX ELEMENTS OF MANY-BODY OPERATORS

Example (motivation):

CI,

$$|\Psi\rangle = \sum_{p_1 < \dots < p_N} c_{p_1 \dots p_N} |\Phi_{p_1 \dots p_N}\rangle$$

$$H|\Psi\rangle = E|\Psi\rangle$$

$c_{p_1 \ldots p_N}$

$$\underset{\sim}{H} \cdot \underset{\sim}{C} = E \, \underset{\sim}{C}$$

$$\langle \Phi_{p_1} \ldots \Phi_{p_N} | H | \Phi_{q_1 \ldots q_N} \rangle$$

$$Z + V \; (+W + \ldots)$$

1-body

2-body

higher than 2-body in various effective Hamiltonians (e.g., nuclear physics)

One-body operators

$$\langle \{p_1 \ldots p_N\} | \hat{Z} | \{q_1 \ldots q_N\} \rangle$$

$$= \sum_{r,s} \langle r | \hat{z} | s \rangle$$

$$\times \langle 0 | X_{p_N} \ldots X_{p_1} X_r^\dagger X_s X_{q_1}^\dagger \ldots X_{q_N}^\dagger | 0 \rangle$$

fully contracted terms
(rule 6)

Suppose X_s contracts $X^\dagger_{q_j}$

Suppose $X^\dagger_r$ contracts X_{p_i}

$$= \sum_{r,s} \langle r | \hat{z} | s \rangle$$

$$\times \langle 0 | X_{p_N} \cdots X_{p_1} X^\dagger_r X_s X^\dagger_{q_1} \cdots X^\dagger_{q_N} | 0 \rangle$$

X_{p_i} $\qquad$ $X^\dagger_{q_j}$

$p_k, k \neq i$ $\qquad$ $q_l, l \neq j$

$\{p_k\}_{k \neq i}$ must be a permutation of $\{q_l\}_{l \neq j}$

or one gets zero.

$|\{p_1 \cdots p_N\}\rangle$ and

$|\{q_1 \cdots q_N\}\rangle$ may differ by at most ONE SPIN-ORBITAL or we get 0.

$\langle\{p_1 \cdots p_N\}|Z|\{q_1 \cdots q_N\}\rangle = 0$ if the two determinants differ by more than one spin-orbital.

We obtain a nonzero result if

1. $\{p_1, \ldots, p_N\}$ and $\{q_1, \ldots, q_N\}$ differ by exactly one index or

2. $\{p_k\}_{k=1}^{N}$ and $\{q_l\}_{l=1}^{N}$ do not differ or differ by a permutation.

① Let us assume that $p_2 = q_2, \dots, p_N = q_N$ but $p_1 \neq q_1$.

$$\langle \{p_1 p_2 \cdots p_N\} | Z | \{q_1 p_2 \cdots p_N\} \rangle$$

$$= \sum_{r,s} \langle r | \hat{z} | s \rangle$$

$$\times \langle 0 | X_{p_N} \cdots X_{p_2} X_{p_1} X_r^\dagger X_s X_{q_1}^\dagger X_{p_2}^\dagger \cdots X_{p_N}^\dagger | 0 \rangle$$

$$= \sum_{r,s} \langle r | \hat{z} | s \rangle \delta_{rp_1} \delta_{sq_1}$$

$$= \langle p_1 | \hat{z} | q_1 \rangle \checkmark$$

2 We can assume that $p_i = q_i$, $i = 1, \ldots, N$

$$\langle \{p_1 \ldots p_N\} | Z | \{p_1 \ldots p_N\} \rangle$$

$$= \sum_{r,s} \langle r | \hat{z} | s \rangle$$

$$\sum_{i=1}^{N} \langle 0 | X_{p_N} \cdots X_{p_i} \cdots X_{p_1} X_r^\dagger X_s X_{p_1}^\dagger \cdots X_{p_i}^\dagger \cdots X_{p_N}^\dagger | 0 \rangle$$

$$= \sum_{r,s} \langle r | \hat{z} | s \rangle \sum_{i=1}^{N} \delta_{r p_i} \delta_{s p_i}$$

$$= \sum_{i=1}^{N} \sum_{r,s} \langle r | \hat{z} | s \rangle \delta_{r p_i} \delta_{s p_i}$$

$$= \sum_{i=1}^{N} \langle p_i | \hat{z} | p_i \rangle \quad \checkmark$$

Two-body operators

Similarly, we can show that

$$\langle \{p_1 \cdots p_N\} | V | \{q_1 \cdots q_N\} \rangle$$

is not zero if

① $\{p_k\}_{k=1}^{N}$ and $\{q_l\}_{l=1}^{N}$ differ by exactly two spin-orbitals,

(2) $\{p_k\}_{k=1}^{N}$ and $\{q_\ell\}_{\ell=1}^{N}$ differ by one spin-orbital, or

(3) $\{p_k\}_{k=1}^{N}$ and $\{q_\ell\}_{\ell=1}^{N}$ do not differ or differ by a permutation.

Repeating the analysis similar to Z, we obtain the following:

① :

$$\langle \{p_1 p_2 p_3 \cdots p_N\} | V | \{q_1 q_2 p_3 \cdots p_N\} \rangle$$

$$= \langle p_1 p_2 | \hat{o} | q_1 q_2 \rangle_A \quad \checkmark$$

② :

$$\langle \{p_1 p_2 \cdots p_N\} | V | \{q_1 p_2 \cdots p_N\} \rangle$$

$$= \sum_{\substack{k=1 \\ (k=2)}}^{N} \langle p_1 p_k | \hat{o} | q_1 p_k \rangle_A \quad \checkmark$$

③ :

$$\langle \{p_1 \dots p_N\} | V | \{p_1 \dots p_N\} \rangle$$

$$= \sum_{1=k<l}^{N} \langle p_k p_l | \hat{v} | p_k p_l \rangle_{A}$$

$$= \frac{1}{2} \sum_{k \neq l}^{N} \langle p_k p_l | \hat{v} | p_k p_l \rangle_{A}$$

$$= \frac{1}{2} \sum_{k,l=1}^{N} \langle p_k p_l | \hat{v} | p_k p_l \rangle_{A}$$

✓

HOLE-PARTICLE FORMALISM

$$\langle \Psi | \hat{O}^{(1)} \dots \hat{O}^{(k)} | \Psi \rangle$$

$$\big\downarrow \qquad\qquad\qquad \big\downarrow$$

$$\langle \Phi_{p_1 \dots p_N} | \, x^\dagger \dots x \, | \Phi_{q_1 \dots q_N} \rangle$$

$$\Downarrow$$

$$\langle 0 | \underbrace{x_{p_N} \dots x_{p_1}}_{N} \, \underbrace{x^\dagger \dots x}_{m} \, \underbrace{x^\dagger_{q_1} \dots x^\dagger_{q_N}}_{N} | 0 \rangle$$

(a lot of operators when N is larger)

$$|\Psi\rangle = \sum_{q_1<\dots<q_N} c_{q_1\dots q_N} \times |\{q_1\dots q_N\}\rangle$$

$$|\Phi\rangle = |\{p_1\dots p_N\}\rangle$$

REFERENCE DETERMINANT

(formally, any determinant that has a nonzero overlap with $|\Psi\rangle$, $\langle\Phi|\Psi\rangle \neq 0$; in practice, the dominant determinant)

We will rebuild the remaining determinants through PARTICLE-HOLE EXCITATIONS (p-h)

Example:

$$|\{p_1 \cdots p_{\mu-1}\, q_\mu\, p_{\mu+1} \cdots p_N\}\rangle$$

$$= X^\dagger_{p_1} \cdots X^\dagger_{p_{\mu-1}}\, X^\dagger_{q_\mu}\, X^\dagger_{p_{\mu+1}} \cdots X^\dagger_{p_N} |0\rangle$$

$$X^{\dagger}_{q_\mu} X_{p_\mu} \underbrace{|\{p_1 \cdots p_{\mu-1}\, \cancel{p_\mu}\, p_{\mu+1} \cdots p_N\}\rangle}_{|\Phi\rangle}$$

$$= X^{\dagger}_{q_\mu} X_{p_\mu} |\Phi\rangle$$

$i, j, k, \ldots$ — single-particle states

HOLE STATES (holes) — OCCUPIED in $|\Phi\rangle$ $(p_1, p_2, \cdots, p_N)$

$a, b, c, \ldots$ – single-particle state

PARTICLE STATES (particles)

UNOCCUPIED in $|\Phi\rangle$

$p, q, r, \ldots$ – generic indices (occ. or unocc.)

singly excited determinant

$$X_a^\dagger X_i |\Phi\rangle = |\Phi_i^a\rangle$$

$$X_a^\dagger X_i X_b^\dagger X_j |\Phi\rangle = |\Phi_{ij}^{ab}\rangle$$

doubly excited determinant

etc.

$$\underbrace{|\Phi_{\overbrace{i_1 \ldots i_n}^{\text{holes}}}^{\overbrace{a_1 \ldots a_n}^{\text{particles}}}\rangle}_{\text{n-tuply excited determinant}} = \prod_{\mu=1}^{n} X_{a_\mu}^{\dagger} X_{i_\mu} |\Phi\rangle$$

$$n = 1, \ldots, N$$

$$|\Psi\rangle = c_0|\Phi\rangle + \sum_{i,a} c_a^i |\Phi_i^a\rangle + \sum_{i<j,\, a<b} c_{ab}^{ij} |\Phi_{ij}^{ab}\rangle \;\checkmark$$

$$+ \ldots = c_0|\Phi\rangle + \sum_{n=1}^{N} \sum_{\substack{i_1<\ldots<i_n \\ a_1<\ldots<a_n}} c_{a_1\ldots a_n}^{i_1\ldots i_n} |\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}\rangle \;\checkmark$$

$$\checkmark \quad C^{i_1 \dots i_n}_{a_1 \dots a_n} = \langle \Phi^{a_1 \dots a_n}_{i_1 \dots i_n} | \Psi \rangle$$

$$|\Phi^{ab}_{ij}\rangle = -|\Phi^{ab}_{ji}\rangle$$

$$= -|\Phi^{ba}_{ij}\rangle = +|\Phi^{ba}_{ji}\rangle$$

$$C^{ij}_{ab} = -C^{ji}_{ab} = -C^{ij}_{ba}$$

$$= C^{ji}_{ba} \quad \left(C^{ii}_{ab} = 0, \; C^{ij}_{aa} = 0 \right)$$

$$|\Psi\rangle = c_0 |\Phi\rangle + \sum_{n=1}^{N} \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1 \neq \dots \neq i_n \\ a_1 \neq \dots \neq a_n}} C^{i_1 \dots i_n}_{a_1 \dots a_n} |\Phi^{a_1 \dots a_n}_{i_1 \dots i_n}\rangle$$

vanish if some i's or a's are identical

$$|\Psi\rangle = c_0 |\Phi\rangle + \sum_{n=1}^{N} \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,\ldots,i_n \\ a_1,\ldots,a_n}} c_{a_1\ldots a_n}^{i_1\ldots i_n} |\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}\rangle$$

allow terms which are zero

the unit operator

$$|\Psi\rangle = (c_0 \hat{1} + \hat{C})|\Phi\rangle$$

$$\hat{C} = \sum_{n=1}^{N} \hat{C}_n$$

$$\hat{C}_n |\Phi\rangle = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,\dots,i_n \\ a_1,\dots,a_n}} c^{i_1\dots i_n}_{a_1\dots a_n} |\Phi^{a_1\dots a_n}_{i_1\dots i_n}\rangle$$

elementary np-nh
excitation operators

$$E^{a_1\dots a_n}_{i_1\dots i_n} = X^\dagger_{a_1} X_{i_1} \cdots X^\dagger_{a_n} X_{i_n}$$

$$E^{a}_{i} = X^\dagger_{a} X_{i} \quad \checkmark$$

$$E^{a_1\dots a_n}_{i_1\dots i_n} = \prod_{\mu=1}^{n} E^{a_\mu}_{i_\mu} \quad \checkmark$$

$$E^{a_1\dots a_n}_{i_1\dots i_n} |\Phi\rangle = |\Phi^{a_1\dots a_n}_{i_1\dots i_n}\rangle$$

$$|\Psi\rangle = (c_0 \mathbb{1} + \hat{C})|\Phi\rangle$$

$$\hat{C} = \sum_{n=1}^{N} \hat{C}_n$$

$$\hat{C}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1 \ldots i_n \\ a_1 \ldots a_n}} c_{a_1 \ldots a_n}^{i_1 \ldots i_n} E_{i_1 \ldots i_n}^{a_1 \ldots a_n}$$

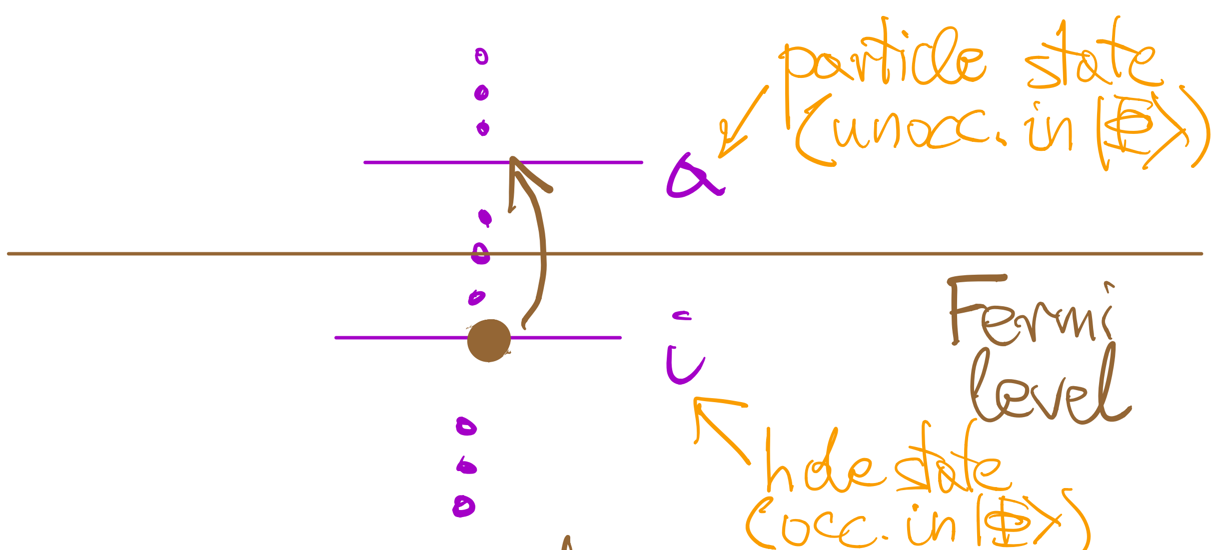
$$X_{a_1}^{\dagger} \ldots X_{a_n}^{\dagger} X_{i_n} \ldots X_{i_1}$$

$$= X_{a_1}^{\dagger} X_{i_1} \ldots X_{a_n}^{\dagger} X_{i_n}$$

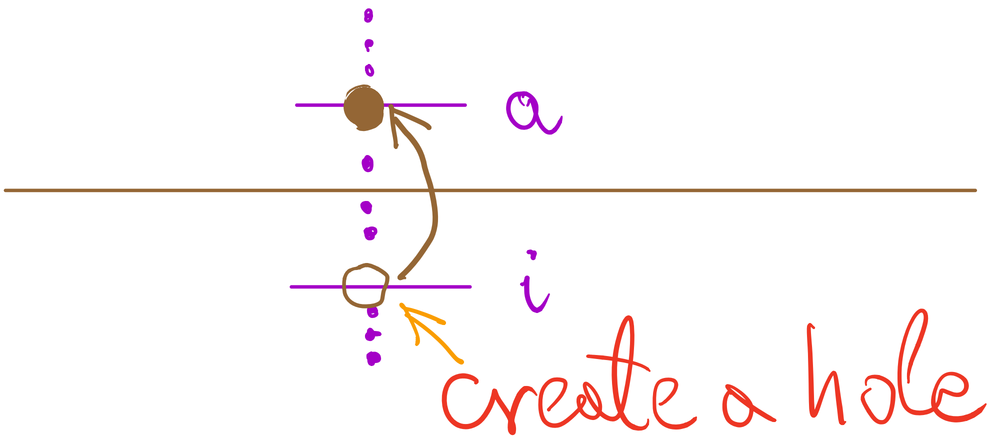
np-nh excitation operator

$$\left(\begin{aligned} &c_0 = 1 \quad (\langle \Phi | \Psi \rangle = 1) \\ &T = \ln(1 + C) \\ &|\Psi\rangle = e^{T} |\Phi\rangle \end{aligned} \right)$$

CC theory



$$\cdots X_a^{\dagger} \cdots X_i \cdots |\Phi\rangle$$



$|\Phi\rangle =$ FERMI VACUUM (STATE)

Examples of benefits:

$$\langle \Phi | V | \Phi_{ij}^{ab} \rangle = \frac{1}{2}\sum_{r,s,t,u} \langle rs | \hat{v} | tu \rangle$$

$$\times \langle \Phi | X_r^\dagger X_s^\dagger X_u X_t X_a^\dagger X_i X_b^\dagger X_j | \Phi \rangle$$

(8 operators, not $2N+8$)

Hole-particle creation and annihilation operators

holes ($i \in$ occ.) $\quad Y_i = X_i^\dagger, \quad Y_i^\dagger = X_i$

particles ($a \in$ unocc.) $\quad Y_a = X_a, \quad Y_a^\dagger = Y_a^\dagger$

$$Y_p = \begin{cases} X_p^\dagger & \text{for } p = i \\ X_p & \text{for } p = a \end{cases}$$

$$Y_p^t = \begin{cases} X_p & \text{for } p = i \\ X_p^t & \text{for } p = a \end{cases}$$

NEXT ...

1. Previously, $X_p |0\rangle = 0. \ \forall p$

Now, $Y_p |\Phi\rangle = 0$

Proof:

$$|\Phi\rangle = |\{1 \ldots N\}\rangle$$

$$i = 1, \ldots, N, \ a = N+1, \ldots$$

$$Y_i|\Phi\rangle = X_i^\dagger|\{1\ldots N\}\rangle$$
$$= 0 \quad (i=1,\ldots,N)$$
$$Y_a|\Phi\rangle = X_a|\{1\ldots N\}\rangle$$
$$= 0. \quad (a=N+1,\ldots)$$

2. $\{Y_p, Y_q\} = 0$

$$\{Y_p^\dagger, Y_q^\dagger\} = 0$$
$$\{Y_p, Y_q^\dagger\} = \delta_{pq}$$
$$(\ldots)$$