WICK's THEOREM

no contractions

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

single contractions

$$+ \sum_{1 \le i < j \le m} n[M_1 \dots M_i \dots M_j \dots M_m]$$

double contractions

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

$$(M_i = X_p \text{ or } X_p^\dagger)$$

Proof of Wick's theorem requires two lemmas.

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):

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

case A (easy) $\leftrightarrow X_r$

$X_r^+ \leftrightarrow$ case B (difficult)

$$n[M_1 \dots M_m] X_r^+$$
$$= n[M_1 \dots M_m X_r^+]$$
$$+ \sum_{i=1}^{m} n[M_1 \dots \underbrace{M_{\bar{i}} \dots M_m}\, X_r^+]$$

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

$\Downarrow$ hard

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

easier

$$\Downarrow$$

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

MUST PROVE

$$\underbrace{n[X_{p_1}\cdots X_{p_m}X_r^{+}] + \sum_{i=1}^{m} n[X_{p_1}\cdots \underbrace{X_{p_i}\cdots X_{p_m}X_r^{+}}_{}]}_{\text{proof by induction}}$$

proof by induction

(videos 6,7)

B2 (proof by reduction to B1, video 7)

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

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

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

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

$$\left(X_{P_{R_1}}^{t} \cdots X_{P_{R_k}}^{t}\right) \cap \left[X_{P_{R_{k+1}}} \cdots X_{P_{R_m}}\right] X_r^{t}$$

$$= \left(X_{P_{R_1}}^{t} \cdots X_{P_{R_k}}^{t}\right) \cap \left[X_{P_{R_{k+1}}} \cdots X_{P_{R_m}} X_r^{t}\right]$$

$$+ \left(X_{P_{R_1}}^{t} \cdots X_{P_{R_k}}^{t}\right) \sum_{i=k+1}^{m} \cap \left[X_{P_{R_{k+1}}} \cdots X_{P_{R_i}} \cdots X_{P_{R_m}} X_r^{t}\right]$$

$\longrightarrow$ case B1

$\therefore$

Lemma 2:

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

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

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

same as on the lhs

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

Proof by reduction to Lemma 1.

PROOF OF WICK'S THEOREM (WT)

(by induction)

m operators : $M_1, \dots, M_m$

Start with $m=1$:

$$M_1 = n[M_1]$$

$m=2$:

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

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

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

(definition of contraction)

Induction step

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

$$M_1 \dots M_\ell M_{\ell+1} = \overset{\text{lemma 1}}{n[M_1 \dots M_\ell] M_{\ell+1}} \quad (1)$$

$$+ \sum_{1 \leq i_1 < j_1 \leq \ell} \overset{\text{lemma 2}}{n[M_1 \dots \underbrace{M_{i_1} \dots M}_{}{}_{j_1} \dots M_\ell] M_{\ell+1}} \quad (2)$$

$$+ \sum_{\substack{i_1 < j_1 \\ i_2 < j_2 \\ i_1 < i_2,\, j_1 \neq j_2}}^{\leq \ell} \overset{\text{lemma 2}}{n[M_1 \dots \underbrace{M_{i_1} \dots M}_{}{}_{j_1} \dots \underbrace{M_{i_2} \dots M}_{}{}_{j_2} \dots M_\ell] M_{\ell+1}} \quad (3)$$

$$+\dots+\left\{\begin{array}{l}\displaystyle\sum_{\dots\, k=1,\ell} n\left[M_1 \dots M_{k-1}\, M_k\, M_{k+1} \dots M_\ell\right] M_{\ell+1} \\ \dots\end{array}\right.$$

lemma 2

odd ℓ

OR

$$(+) \sum_{\dots} n\left[M_1 \dots M_\ell\right] M_{\ell+1}$$

fully contracted (f.c.)

even ℓ

$$= n\left[M_1 \dots M_\ell\, M_{\ell+1}\right] \quad ①$$

$$+ \sum_{k=1}^{\ell} n\left[M_1 \dots M_k \dots M_\ell\, M_{\ell+1}\right] \quad ①$$

$$\Updownarrow$$

$$+ \sum_{1 \le i_1 < j_1 \le \ell} n\left[M_1 \dots M_{i_1} \dots M_{j_1} \dots M_\ell\, M_{\ell+1}\right] \quad ②$$

$$+\sum_{\substack{i_1<j_1\\ k=1,\dots,l,\ \leq l\\ k\neq i_1,j_1}} n[M_1\cdots \underbrace{M_{i_1}\cdots}\, M_{j_1}\cdots \underbrace{M_k\cdots M_l}\, M_{l+1}] \qquad ②$$

$$\Updownarrow$$

$$+\sum_{\substack{i_1<j_1\\ i_2<j_2\\ i_1<i_2,\ j_1\neq j_2}} \leq l \quad n[M_1\cdots \underbrace{M_{i_1}\cdots}\, M_{j_1}\cdots \underbrace{M_{i_2}\cdots}\, M_{j_2}\cdots M_l\, M_{l+1}] \qquad ③$$

$$+\sum_{\substack{i_1<j_1\\ i_2<j_2\\ i_1<i_2,\ j_1\neq j_2\\ k\neq i_1,j_1,i_2,j_2}} \leq l \quad n[M_1\cdots \underbrace{M_{i_1}\cdots}\, M_{j_1}\cdots \underbrace{M_k\cdots \underbrace{M_{i_2}\cdots}\, M_{j_2}\cdots M_l}\, M_{l+1}] \qquad ③$$

$$\Updownarrow$$

$$+\cdots$$

$$= n[M_1 \dots M_\ell M_{\ell+1}] \qquad \checkmark$$

$$+ \sum_{1 \le i_1 < j_1 \le \ell+1} n[M_1 \dots \underbrace{M_{i_1} \dots M_{j_1}} \dots M_\ell \, M_{\ell+1}] \qquad \checkmark$$

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

$$+ \dots$$

$$\therefore$$

GENERALIZED WICK'S THEOREM (GWT)

Example:

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

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

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

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

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

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

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

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

normal products involving $M_1 M_2$ and/or $M_3 M_4$ do not contribute

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

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

$$+ \sum_{i_1 < j_1}{}' \, n[M_1 \dots M_{i_1} \dots M_{j_1} \dots M_m]$$

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

$$+ \ldots$$

$\sum'$ $\rightarrow$ exclude contractions involving operators that originate from the same normal product

Proof by reduction to WT and recognition that

$\underbrace{X^\dagger X}_{}$, $\underbrace{X^\dagger X^\dagger}_{}$, and $\underbrace{XX}_{}$ are all zero.

Rules 1–4:

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

$(\sqcup\!\sqcup) \leftarrow$ without or with contractions

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

$(\sqcup\!\sqcup) \leftarrow$ without or with contractions

Rules 5–7:

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

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

Rule 5:

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

(use WT and rules 2 and 4')

Rule 6:

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

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

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

+/-

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

(use WT and rule 2 and 4)

Rule 7:

$$M_1 \dots M_m |0\rangle$$

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

(annihilators fully contracted)

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

indices of contracted operators

(use WT and rules 1 and 3)

Example:

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

rule 6

$$= \langle 0 | n[X_p X_q^\dagger X_r X_s^\dagger] | 0 \rangle$$

f.c.

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

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

(also GWT)

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

Verification:

$$X_p \overbrace{X_q^\dagger X_r}^{n[X_q^\dagger X_r]} X_s^\dagger$$

$$\begin{aligned}
\overset{\text{GWT}}{=} & - X_q^\dagger X_s^\dagger X_p X_r && n[X_p X_q^\dagger X_r X_s^\dagger] \\
& - \delta_{pq} X_s^\dagger X_r && n[X_p X_q^\dagger X_r X_s^\dagger] \\
& + \delta_{ps} X_q^\dagger X_r && n[X_p X_q^\dagger X_r X_s^\dagger] \\
& - \delta_{rs} X_q^\dagger X_p && n[X_p X_q^\dagger X_r X_s^\dagger] \\
& + \delta_{pq} \delta_{rs} && n[X_p X_q^\dagger X_r X_s^\dagger]
\end{aligned}$$

$$\langle 0 | X_p X_q^\dagger X_r X_s^\dagger | 0 \rangle = \delta_{pq} \delta_{rs}$$

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

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

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

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

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

$$\overset{\text{rule 6}}{=} \sum_{\text{f.c.}} \langle 0 | n[X_{p_N} \dots X_{p_1} X^{\dagger}_{q_1} \dots X^{\dagger}_{q_N}] |0\rangle$$

$$= \sum_{R \in S_N} (-1)^R \langle 0 | n \left[X_{p_N} \cdots X_{p_2} X_{p_1} X^\dagger_{q_{R_1}} X^\dagger_{q_{R_2}} \cdots X^\dagger_{q_{R_N}} \right] | 0 \rangle$$

$$= \sum_{R \in S_N} (-1)^R \overbrace{\langle p_1 | q_{R_1} \rangle}^{\delta_{p_1 q_{R_1}}} \overbrace{\langle p_2 | q_{R_2} \rangle}^{\delta_{p_2 q_{R_2}}} \times \cdots \times \underbrace{\langle p_N | q_{R_N} \rangle}_{\delta_{p_N q_{R_N}}}$$

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

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

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

MATRIX ELEMENTS OF MANY-BODY OPERATORS

Motivation: Configuration Interaction (CI)

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

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

$c_{q_1\dots q_N}$

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

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

$$Z + V \quad (+W+\dots)$$

1-body

2-body

3-body and other higher-than-2-body in various effective Hamiltonians

One-body operators

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

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

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

fully contracted terms (rule 6)

Suppose X_s is contracted with $X_{q_j}^\dagger$

Suppose $X_r^\dagger$ is contracted with X_{p_i}

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

$$\times \langle 0| \underbrace{X_{p_N} \cdots X_{p_1}}_{X_{p_i}} X_r^\dagger \; X_s \underbrace{X_{q_1}^\dagger \cdots X_{q_N}^\dagger}_{X_{q_j}^\dagger} |0\rangle$$

X_{p_k}, $k \neq i$ must be contracted with $X_{q_\ell}^\dagger$, $\ell \neq j$.

$$\Downarrow$$

$\{p_k\}_{k\neq i}$ must be a permutation of $\{q_\ell\}_{\ell \neq j}$ or one gets a zero.

$|\{p_1 \ldots p_N\}\rangle$ and $|\{q_1 \ldots q_N\}\rangle$ may differ by at most ONE single-particle state.

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

$= 0$ if the two determinants differ by more than one single-particle state (spin-orbital).

We obtain a nonzero result if

1. $\{p_1, \cdots, p_N\}$ and $\{q_1, \cdots, q_N\}$ 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 $p_1 \neq q_1$.

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

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

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

$$= \sum_{r,s} \langle r | \hat{z} | s \rangle \delta_{r p_1} \delta_{s q_1}$$

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

(2) We can assume that $p_i = q_i$, $i = 1, \dots, N$

$$\langle \{p_1 \dots p_N\} | \hat{Z} | \{p_1 \dots p_N\} \rangle$$

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

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

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

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

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

Two-body operators

Similarly, we can show that

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

is not zero if

1. $\{p_k\}_{k=1}^N$ and $\{q_l\}_{l=1}^N$ differ by exactly two single-particle states,

2. $\{p_k\}_{k=1}^N$ and $\{q_l\}_{l=1}^N$ differ by exactly one single-particle state, or

③ $\{p_k\}_{k=1}^N$ and $\{q_l\}_{l=1}^N$ do not differ or differ by a permutation.

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

① $\langle\{p_1 p_2 p_3 \cdots p_N\}|V|\{q_1 q_2 p_3 \cdots p_N\}\rangle$

$= \langle p_1 p_2 | \hat{v} | q_1 q_2 \rangle_{CA}$

② $\langle\{p_1 p_2 \cdots p_N\}|V|\{q_1 p_2 \cdots p_N\}\rangle$

$= \sum_{\substack{k=2 \\ (k=1)}}^{N} \langle p_1 p_k | \hat{v} | q_1 p_k \rangle_{CA}$

$\langle p_1 p_1 | \hat{v} | q_1 p_1 \rangle_{CA} = 0$

3

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

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

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

$$= \frac{1}{2} \sum_{k,l=1}^{N} \langle p_k p_l | \hat{v} | p_k p_l \rangle_A \qquad \langle p_k p_k | \hat{v} | p_k p_k \rangle_A = 0$$

video 10