① $\{X_p^+, X_q\} = X_p^+ X_q + X_q X_p^+$
$= \delta_{pq}$

② $\{X_p, X_q\} = X_p X_q + X_q X_p = 0$

③ $\{X_p^+, X_q^+\} = X_p^+ X_q^+ + X_q^+ X_p^+ = 0$

①

$p \neq q \;, \quad p = q$

$p < q \qquad p > q$

✓ $\underline{p < q}$:

✓ $\{X_p^+, X_q\} |\ldots \cancel{p} \ldots \cancel{q} \ldots\rangle$

$= X_p^+ X_q |\ldots \cancel{p} \ldots \cancel{q} \ldots\rangle$

$+ X_q X_p^+ |\overbrace{\ldots}^{m} \cancel{p} \ldots \cancel{q} \ldots\rangle$

m = the number of occupied single-particle states before p

$$= 0 + X_q (-1)^m |\ldots p \ldots \cancel{q} \ldots\rangle$$

$$= 0$$

the number of occupied single-particle states between p and q

$$\checkmark \quad \{X_p^\dagger, X_q\} |\overbrace{\ldots}^{m} \cancel{p} \overbrace{\ldots}^{n} q \ldots\rangle$$

$$= X_p^\dagger X_q |\overbrace{\ldots}^{m} \cancel{p} \overbrace{\ldots}^{n} q \ldots\rangle$$

$$+ X_q X_p^\dagger |\overbrace{\ldots}^{m} \cancel{p} \overbrace{\ldots}^{n} q \ldots\rangle$$

$$= X_p^\dagger (-1)^{m+n} |\overbrace{\ldots}^{m} \cancel{p} \ldots \cancel{q} \ldots\rangle$$

$$+ X_q (-1)^m |\overbrace{\ldots}^{m} p \overbrace{\ldots}^{n} q \ldots\rangle$$

$$= (-1)^{\cancel{m}+n} (-1)^{\cancel{m}} |\ldots p \ldots \cancel{q} \ldots\rangle$$

$$+ (-1)^{\cancel{m}} (-1)^{\cancel{m}+n+1} |\ldots p \ldots \cancel{q} \ldots\rangle$$

$$= \underbrace{\left[(-1)^n + (-1)^{n+1}\right]}_{(-1)^n[1-1] = 0} |\ldots p \ldots \cancel{q} \ldots\rangle$$

$$= 0.$$

$$\checkmark \quad \{X_p^\dagger, X_q\} |\ldots p \ldots \cancel{q} \ldots\rangle$$

$$= X_p^\dagger X_q |\ldots p \ldots \cancel{q} \ldots\rangle$$

$$+ X_q X_p^\dagger |\ldots p \ldots \cancel{q} \ldots\rangle$$

$$= 0 + 0 = 0$$

$$\checkmark \quad \{X_p^\dagger, X_q\} |\ldots p \ldots q \ldots\rangle$$

$$= X_p^\dagger X_q |\overbrace{\ldots}^{m} p \overbrace{\ldots}^{n} q \ldots\rangle$$

$$+ X_q X_p^\dagger |\overbrace{\ldots}^{m} p \overbrace{\ldots}^{n} q \ldots\rangle$$

$$= \ldots \quad 0$$

$$\boxed{\begin{gathered}\{X_p, X_q^\dagger\} = 0 \\ p<q,\ p>q\end{gathered}}$$

$p=q$:

$$\checkmark\ \{X_p^\dagger, X_p\}|\ldots p \ldots\rangle$$

$$= X_p^\dagger X_p |\overbrace{\ldots}^{m} p \ldots\rangle$$

$$+ X_p X_p^\dagger |\overbrace{\ldots}^{m} p \ldots\rangle$$

$$= X_p^\dagger (-1)^m |\overbrace{\ldots}^{m} \cancel{p} \ldots\rangle + 0$$

$$= (-1)^m (-1)^m |\ldots p \ldots\rangle$$

$$= |\ldots p \ldots\rangle$$

$$\checkmark \quad \{X_p^\dagger, X_p\}|\ldots\cancel{p}\ldots\rangle$$

$$= X_p^\dagger X_p|\ldots\cancel{p}\ldots\rangle$$

$$+ X_p X_p^\dagger|\overbrace{\ldots}^{m}\cancel{p}\ldots\rangle$$

$$= 0 + (-1)^m X_p|\overbrace{\ldots}^{m}p\ldots\rangle$$

$$= (-1)^m(-1)^m|\ldots\cancel{p}\ldots\rangle$$

$$= |\ldots\cancel{p}\ldots\rangle$$

$$\{X_p^\dagger, X_p\} = \mathbb{1}$$

$$\{X_p^\dagger, X_q\} = \delta_{pq}\mathbb{1}$$

$$= \delta_{pq}.$$

- $$X_p^2 = 0, \quad (X_p^\dagger)^2 = 0$$

(nilpotent)

Proof:

$$0 = \{X_p, X_p\} = X_p X_p + X_p X_p$$
$$= 2X_p^2$$
$$X_p^2 = 0.$$

Similarly for $X_p^\dagger$.

- $$X_p X_q = -X_q X_p$$
$$X_p^\dagger X_q^\dagger = -X_q^\dagger X_p^\dagger$$

In general,

$$X_{p_{R_1}} \cdots X_{p_{R_N}} = (-1)^R X_{p_1} \cdots X_{p_N}$$

$$R = \begin{pmatrix} 1 & \dots & N \\ R_1 & \dots & R_N \end{pmatrix}$$

Similarly for $X^\dagger$'s.

- $N_p^2 = N_p$ (idempotent)

  $N_p = X_p^\dagger X_p$ $(N_p^\dagger = N_p)$

  $N_p |\dots n_p \dots\rangle = n_p |\dots n_p \dots\rangle,$

  $n_p = 0, 1.$

- $[N_p, N_q] = 0.$

- $$[X_p, N_q] = \delta_{pq} X_p$$
$$[X_p^\dagger, N_q] = -\delta_{pq} X_p^\dagger$$

Example:

$$\langle \Phi_{pq} | \Phi_{rs} \rangle = \langle \{pq\} | \{rs\} \rangle = \begin{vmatrix} \langle p|r\rangle & \langle p|s\rangle \\ \langle q|r\rangle & \langle q|s\rangle \end{vmatrix} = \begin{vmatrix} \delta_{pr} & \delta_{ps} \\ \delta_{qr} & \delta_{qs} \end{vmatrix}$$

$$|\Phi_{pq}\rangle \equiv |\{pq\}\rangle = X_p^\dagger |\{q\}\rangle = X_p^\dagger X_q^\dagger |0\rangle$$

$$|\Phi_{rs}\rangle = \chi_r^\dagger \chi_s^\dagger |0\rangle$$

$$\langle \Phi_{pq}|\Phi_{rs}\rangle =$$

try to relocate to the right most position, since $\chi_p|0\rangle = 0$

$$= \langle 0|\chi_q \chi_p \chi_r^\dagger \chi_s^\dagger|0\rangle$$

$$= \langle 0|\chi_q (\delta_{pr} - \chi_r^\dagger \chi_p) \chi_s^\dagger|0\rangle$$

$$= \delta_{pr} \langle 0|\chi_q \chi_s^\dagger|0\rangle$$

$$- \langle 0|\chi_q \chi_r^\dagger \chi_p \chi_s^\dagger|0\rangle$$

$$= \langle p|r\rangle \langle q|s\rangle$$

$$- \langle 0|\chi_q \chi_r^\dagger (\delta_{ps} - \chi_s^\dagger \chi_p)|0\rangle$$

$$= \langle p|r\rangle \langle q|s\rangle$$

$$- \langle 0 | X_q X_r^\dagger | 0 \rangle \delta_{ps}$$

$$+ \langle 0 | X_q X_r^\dagger X_s^\dagger \underbrace{X_p | 0 \rangle}_{=0}$$

$$= \langle p | r \rangle \langle q | s \rangle - \langle q | r \rangle \langle p | s \rangle$$

$$= \begin{vmatrix} \langle p | r \rangle & \langle p | s \rangle \\ \langle q | r \rangle & \langle q | s \rangle \end{vmatrix}$$

$$\langle \Phi_{pq} | \Phi_{rs} \rangle = \delta_{pr} \delta_{qs}$$

$p < q$, $r < s$

OPERATORS IN SECOND QUANTIZATION

$$\hat{O} = \sum_{k=0}^{N} \hat{O}_k$$

k-body component of $\hat{O}$

$$\hat{O}_k = \sum_{1=i_1<\dots<i_k}^{N} \hat{o}_k(x_{i_1},\dots,x_{i_k})$$

Examples:

$k=1$

$$\hat{Z} = \sum_{i=1}^{N} \hat{z}(x_i)$$

$k=2$

$$\hat{V} = \sum_{1=i<j}^{N} \hat{v}(x_i,x_j)$$

$$\hat{H} = \hat{Z} + \hat{V}$$ ← example of $\hat{O} = \hat{O}_1 + \hat{O}_2$

Proof of the second-quantized forms of many-body operators requires four lemmas.

Lemma 1:

$|\Phi_{p_1 \dots p_N}\rangle$

$$|\{p_1 \dots p_N\}\rangle = X^\dagger_{p_1} \dots X^\dagger_{p_N} |0\rangle$$

$$p_1 < \dots < p_N$$ (ordered p's)

Lemma 2:

$$|\{q_1 \dots q_N\}\rangle = X^\dagger_{q_1} \dots X^\dagger_{q_N} |0\rangle$$

q's ordered or not

$|\Phi_{q_1 \dots q_N}\rangle$

Isomorphism

$$\Phi_{p_1 \cdots p_N}(x_1, \ldots, x_N)$$

$$\Updownarrow$$

$$X^{+}_{p_1} \cdots X^{+}_{p_N} |0\rangle$$

Lemma 3:

$$X_q X^{+}_{p_1} \cdots X^{+}_{p_N} |0\rangle$$

$$= \sum_{i=1}^{N} (-1)^{i-1} \delta_{q p_i}$$

$$\times X^{+}_{p_1} \cdots X^{+}_{p_{i-1}} X^{+}_{p_{i+1}} \cdots X^{+}_{p_N} |0\rangle$$

$$\prod X^\dagger |0\rangle = X^\dagger_{p_1} \ldots X^\dagger_{p_N} |0\rangle$$

$$\prod^{p_i} X^\dagger |0\rangle =$$

X_{p_i} removed

$$= X^\dagger_{p_1} \ldots X^\dagger_{p_{i-1}} X^\dagger_{p_{i+1}} \ldots X^\dagger_{p_N} |0\rangle$$

$$X_q \prod X^\dagger |0\rangle$$

$$= \sum_{i=1}^{N} (-1)^{i-1} \delta_{q p_i} \prod^{p_i} X^\dagger |0\rangle$$

Lemma 4:

$$X_r X_s \prod X^\dagger |0\rangle$$

$$= \sum_{1=i<j}^{N} (-1)^{i+j} \delta_{r p_i} \delta_{s p_j} \times \prod^{p_i p_j} X^\dagger |0\rangle \quad ✓$$

$$+ \sum_{i>j=1}^{N} (-1)^{i+j-1} \delta_{r p_i} \delta_{s p_j} \times \prod^{p_i p_j} X^\dagger |0\rangle \quad ✓$$

$$\prod^{p_i p_j} X^\dagger |0\rangle = X^\dagger_{p_1} \cdots \cancel{X^\dagger_{p_i}} \cdots \cancel{X^\dagger_{p_j}} \cdots X^\dagger_{p_N} |0\rangle, \; i<j$$

$$\prod^{p_i p_j} X^\dagger |0\rangle = X^\dagger_{p_1} \cdots \cancel{X^\dagger_{p_j}} \cdots \cancel{X^\dagger_{p_i}} \cdots X^\dagger_{p_N} |0\rangle, \; i>j$$

Main part:

1-body: $$\hat{O}_1 = \sum_{i=1}^{N} \hat{o}_1(x_i)$$

$$\Downarrow$$

$$\hat{O}_1 = \sum_{p,q} \langle p|\hat{o}_1|q\rangle X_p^{\dagger} X_q$$

$$\langle p|\hat{o}_1|q\rangle = \int \chi_p^*(x)\,\hat{o}_1(x)\,\chi_q(x)\,dx$$

2-body: $$\hat{O}_2 = \sum_{1=i<j}^{N} \hat{o}_2(x_i, x_j)$$

$$\Downarrow$$

$$\hat{O}_2 = \frac{1}{2} \sum_{pq,r,s} \langle pq|\hat{o}_2|rs\rangle$$

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

$$\langle pq|\hat{o}_2|rs\rangle = \int \psi_p^*(x_1)\psi_q^*(x_2)$$

$$\times \quad \hat{o}_2(x_1, x_2)\psi_r(x_1)\psi_s(x_2)\,dx_1\,dx_2$$

p	q	$\langle p\|\hat{o}_1\|q\rangle$
1	1	$\langle 1\|\hat{o}_1\|1\rangle$
1	2	$\langle 1\|\hat{o}_1\|2\rangle$

...

k-body: $$\hat{O}_k = \sum_{1=i_1<\dots<i_k}^{N} \hat{o}_k(x_{i_1},\dots,x_{i_k})$$

$\checkmark$

$$\Downarrow$$

$$\hat{O}_k = \frac{1}{k!} \sum_{\substack{p_1\dots p_k \\ q_1\dots q_k}} \langle p_1\dots p_k|\hat{o}_k|q_1\dots q_k\rangle$$

$$\times\, X^{+}_{p_1}\dots X^{+}_{p_k} X_{q_k}\dots X_{q_1}$$

$$\langle p_1\dots p_k|\hat{o}_k|q_1\dots q_k\rangle$$

$$= \int \psi^{*}_{p_1}(x_1)\dots\psi^{*}_{p_k}(x_k) \quad (dx_1\dots dx_k$$

$$\times\ \hat{o}_k(x_1,\dots,x_k)\,\psi_{q_1}(x_1)\dots\psi_{q_k}(x_k))$$

Proof for 1-body:

$$\hat{O}_1 |\Phi_{p_1 \dots p_N}\rangle$$

$$= \sqrt{N!}\, \hat{O}_1 A \prod_{k=1}^{N} \psi_{p_k}(x_k)$$

$\hat{O}_1$ and A commute

In general,

$$[\hat{O}_k, R] = 0 \quad \forall\, R \in S_N$$

$$= \sqrt{N!}\, A \sum_{i=1}^{N} \hat{o}_1(x_i) \prod_{k=1}^{N} \psi_{p_k}(x_k)$$

$$\cdots$$

$$= \sum_{i=1}^{N} \sum_{p} \langle p|\hat{O}_1|p_i\rangle$$

$$\times \,|\Phi_{p_1 \cdots p_{i-1}\, p\, p_{i+1} \cdots p_N}\rangle$$

$$\hat{O}_1\, X^\dagger_{p_1} \cdots X^\dagger_{p_N}|0\rangle = \prod X^\dagger|0\rangle$$

$$= \sum_{i} \sum_{p} \langle p|\hat{O}_1|p_i\rangle$$

$$\times\, \underbrace{X^\dagger_{p_1} \cdots X^\dagger_{p_{i-1}}\, X^\dagger_{p}\, X^\dagger_{p_{i+1}} \cdots X^\dagger_{p_N}|0\rangle}_{(-1)^{i-1} X^\dagger_p \prod^{p_i} X^\dagger|0\rangle}$$

$\ldots$ (lemma 3)

$$= \sum_{pq} \langle p|\hat{o}_1|q\rangle X_p^\dagger X_q \prod X^\dagger |0\rangle$$

$$\hat{O}_1 = \sum_{pq} \langle p|\hat{o}_1|q\rangle X_p^\dagger X_q$$

Similarly for 2-body and k-body with $k>2$.

Alternative forms using antisymmetrized matrix elements.

2-body

$$\hat{O}_2 = \frac{1}{2}\sum_{pq,rs} \langle pq|\hat{o}_2|rs\rangle \times X_p^\dagger X_q^\dagger X_s X_r$$

$$= \frac{1}{4}\sum_{pq,rs} \langle pq|\hat{o}_2|rs\rangle_A \times X_p^\dagger X_q^\dagger X_s X_r$$

anti-symmetrized matrix element

$$\langle pq|\hat{o}_2|rs\rangle_A = \langle pq|\hat{o}_2|rs\rangle - \langle pq|\hat{o}_2|sr\rangle$$

$$\hat{O}_k = \left(\frac{1}{k!}\right)^2$$

antisymmetrized matrix element

$$\times \sum_{\substack{p_1 \cdots p_k \\ q_1 \cdots q_k}} \langle p_1 \cdots p_k | \hat{o}_k | q_1 \cdots q_k \rangle_A$$

$$\times X^\dagger_{p_1} \cdots X^\dagger_{p_k} X_{q_k} \cdots X_{q_1}$$

$$\langle p_1 \cdots p_k | \hat{o}_k | q_1 \cdots q_k \rangle_A$$

$$= \sum_{R \in S_k} (-1)^R \langle p_1 \cdots p_k | \hat{o}_k | q_{R_1} \cdots q_{R_k} \rangle$$

sign of permutation

$$R = \begin{pmatrix} 1 & \cdots & k \\ R_1 & \cdots & R_k \end{pmatrix}$$

SPIN-INDEPENDENT OPERATORS

$$\hat{H} = \sum_{i=1}^{N} \hat{z}(x_i) + \sum_{i<j}^{N} v(x_i, x_j)$$

$$\hat{z}(x_i) = -\frac{1}{2}\Delta_i + \sum_{A=1}^{M} \frac{Z_A}{r_{iA}}$$

$$\hat{v}(x_i, x_j) = \frac{1}{r_{ij}}$$

orbital

$$\psi_p(x,y,z,s) = \varphi_p(x,y,z) \times \sigma(s)$$

spin-orbital

spin function

$$|P\alpha\rangle = |P\rangle \otimes |\alpha\rangle$$

$$|P\beta\rangle = |P\rangle \otimes |\beta\rangle$$

$\uparrow\downarrow \; P$

$$\{ X_{P\sigma_P}, X^\dagger_{Q\sigma_Q} \}$$

$$= \delta_{PQ} \, \delta_{\sigma_P \sigma_Q}$$

$$\hat{O}_1 = \sum_{pq} \langle p | \hat{o}_1 | q \rangle X^\dagger_p X_q$$

...

$$= \sum_{P,Q} \langle P | \hat{o}_1 | Q \rangle$$

$$\times \quad E_{PQ}$$

generators of $U(n)$

number of orbitals

$$E_{PQ} = \sum_{\sigma=-\frac{1}{2}}^{+\frac{1}{2}} X^\dagger_{P\sigma} X_{Q\sigma}$$

$$= X^\dagger_{P\alpha} X_{Q\alpha} + X^\dagger_{P\beta} X_{Q\beta}$$

$$[E_{PQ}, E_{RS}] \quad \checkmark$$

$$= \delta_{QR} E_{PS} - \delta_{PS} E_{RQ}$$

$GL(n)$

$$E_{ij} = \begin{array}{cl} & \downarrow j\text{th column} \\ \begin{bmatrix} 0 & \cdots & 0 \\ \vdots & 1 & \vdots \\ 0 & \cdots & 0 \end{bmatrix} & \leftarrow i\text{th row} \end{array}$$

$$(E_{ij})_{kl} = \delta_{ik}\delta_{jl}$$

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ & \cdots & \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} = \sum_{i,j=1}^{n} a_{ij} E_{ij}$$

Josef Paldus, 1974

$$\text{UGA} \xrightarrow[\text{Isaiah Shavitt}]{} \text{GUGA}$$

WICK's THEOREM

Motivation:

$$\langle \Psi | \hat{O}_k | \Psi' \rangle$$

$$\langle \Phi_{p_1 \cdots p_N} | \hat{O}_k | \Phi_{q_1 \cdots q_k} \rangle$$

$$\frac{1}{k!} \sum_{\substack{r_1 \cdots r_k \\ s_1 \cdots s_k}} \langle r_1 \cdots r_k | \hat{O}_k | s_1 \cdots s_k \rangle$$

$$\times \langle 0 | \overbrace{X_{p_N} \cdots X_{p_1}}^{\text{from } \langle \Phi_{p_1 \cdots p_N} |} X^{\dagger}_{r_1} \cdots X^{\dagger}_{r_k}$$

$$\times X_{s_k} \cdots X_{s_1} \underbrace{X^{\dagger}_{q_1} \cdots X^{\dagger}_{q_k}}_{\text{from } | \Phi_{q_1 \cdots q_k} \rangle} | 0 \rangle$$

To handle the above expressions, we must learn how to calculate

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

$$M_i = X_{p_i} \text{ or } X^{+}_{p_i}$$

Another typical situation:

$$\hat{O}_k | \Psi \rangle$$

$$\downarrow$$

$$\hat{O}_k | \Phi_{p_1 \ldots p_k} \rangle$$

$$\downarrow$$

$$M_1 \ldots M_m | 0 \rangle,$$

$$M_i = X_{p_i} \text{ or } X^{+}_{p_i}$$

Wick's theorem requires

- normal products ✓
- contractions ✓
- normal products with contractions ✓

Normal products:

$$n\left[M_1 \dots M_m\right] = (-1)^R$$

$$\times X^{+}_{R_1} \dots X^{+}_{R_j} X_{R_{j+1}} \dots X_{R_m}$$

$$R = \begin{pmatrix} 1 & 2 & \dots & j & j+1 & \dots & m \\ R_1 & R_2 & \dots & R_j & R_{j+1} & \dots & R_m \end{pmatrix}$$

$$n[\emptyset] = \mathbb{1}$$

1. $$n[M] = M$$

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

In particular,

$$n[X^+_{p_1} \cdots X^+_{p_j} X_{p_{j+1}} \cdots X_{p_m}] = X^+_{p_1} \cdots X^+_{p_j} X_{p_{j+1}} \cdots X_{p_m}$$

$$n[X^+_{p_1} \cdots X^+_{p_m}] = X^+_{p_1} \cdots X^+_{p_m}$$

$$n[X_{p_1} \cdots X_{p_m}] = X_{p_1} \cdots X_{p_m}$$

3. $$n[M_{R_1} \dots M_{R_m}] = (-1)^R \, n[M_1 \dots M_m]$$

sign of R

$$R = \begin{pmatrix} 1 & \dots & m \\ R_1 & \dots & R_m \end{pmatrix}$$

$$n[M_2 M_1] = -n[M_1 M_2]$$

Contractions:

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

$$M_i = X_{p_i} \text{ or } X^\dagger_{p_i}$$

$$\underbrace{X_p X^\dagger_q}_{} = \delta_{pq}$$ ✓

$$\underbrace{X_p X_q}_{} = 0$$

$$\underbracket{x_p^\dagger x_q} = 0$$

$$\underbracket{x_p^\dagger x_q^\dagger} = 0$$

Normal products with contractions:

$$n[M_1 \dots M_{i_1} \dots M_{i_\lambda} \dots M_{j_1} \dots M_{j_\lambda} \dots M_m]$$

$$= (-1)^R \underbracket{M_{i_1} M_{j_1}} \dots \underbracket{M_{i_\lambda} M_{j_\lambda}}$$

$$\times\, n[M_{k_1} \dots M_{k_\mu}]$$

$$2\lambda + \mu = m$$

(λ contractions in $n[\dots]$; $\lambda \geq 1$)

$$R = \begin{pmatrix} 1 & 2 & \cdots & (2\lambda-1) & (2\lambda) & (2\lambda+1) & \cdots & m \\ i_1 & j_1 & \cdots & i_\lambda & j_\lambda & k_1 & \cdots & k_\mu \end{pmatrix}$$

Observations:

✓ $n[\dots \underbrace{M_i M_{i+1}} \dots]$

$= + \underbrace{M_i M_{i+1}} \, n[\dots]$

✓ In the case of fully contracted expressions, the sign is

$$(-1)^\nu ,$$

where ν is the number of intersections of contraction lines.

$$n[X_p X_q X_r^\dagger X_s X_t^\dagger X_u^\dagger]$$

$\nu = 2$, sign is $(-1)^2 = +1$

$$R = \begin{pmatrix} p & q & r & s & t & u \\ p & r & q & t & s & u \end{pmatrix} = \overset{+}{(p)}\overset{-}{(qr)}\overset{-}{(st)} \times \overset{+}{(u)}$$

$$= + X_p X_r^\dagger X_q X_t^\dagger X_s X_u^\dagger$$

$$\times\, n[\emptyset]$$

This also applies to a situation where contracted operators are grouped together.

Wick's theorem will be:

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

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

$+ \ldots$

We already determined that we need to learn how to calculate

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

and

$$M_1 \ldots M_m | 0 \rangle$$

Rules 1–4 (4')

Rule 1:

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

unless all operators M are creators.

Rule 2:

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

as long as $m \geq 1$.

Rule 3:

$$n[M_1 \ldots M_i \ldots M_j \ldots M_m] | 0 \rangle = 0$$

if at least one uncontracted operator among Ms is an annihilator.

Rule 4:

$$\langle 0 | n[M_1 \ldots M_i \ldots M_j \ldots] | 0 \rangle$$

$= 0$ unless all operators are fully contracted.

Rule 4':

$$\langle 0| n[M_1 \cdots M_i \cdots M_j \cdots M_{2m+1}] |0\rangle = 0.$$

Intro to Wick's theorem:

Calculate $\langle 0| M_1 M_2 |0\rangle$, $M_i = X_{p_i}$ or $X^\dagger_{p_i}$

Conventional method:

$$\langle 0| X_p X_q |0\rangle = 0$$

$$\langle 0| X_p X_q^\dagger |0\rangle = \langle p|q\rangle = \delta_{pq}$$

$$\langle 0| X_p^\dagger X_q |0\rangle = 0$$

$$\langle 0| X_p^\dagger X_q^\dagger |0\rangle = 0$$

$\langle 0|M_1 M_2|0\rangle = 0$ unless $M_1 = X_p$ and $M_2 = X_p^\dagger$, in which case we obtain 1.

Alternatively, $M_1 M_2 = n[M_1 M_2] + \underbracket{M_1 M_2}$

$$\begin{aligned}
&\langle 0|M_1 M_2|0\rangle \\
&= \underbrace{\langle 0|n[M_1 M_2]|0\rangle}_{0\ (\text{rule}\ 2)} \\
&\quad + \langle 0|\underbracket{M_1 M_2}|0\rangle \\
&= \underbracket{M_1 M_2}\,\langle 0|0\rangle = \underbracket{M_1 M_2}
\end{aligned}$$

The only nonzero $\underbracket{M_1 M_2}$ is $\underbracket{X_p X_p^\dagger} = 1$.

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

this is Wick's theorem for $m=2$

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

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

Example (out of many):

$$X_p X_q^\dagger X_r^\dagger = n[X_p X_q^\dagger X_r^\dagger]$$

$$+ n[\underbrace{X_p X_q^\dagger} X_r^\dagger]$$

$$+ n[\underbrace{X_p X_q^\dagger X_r^\dagger}]$$

(we can skip $n[X_p \underbrace{X_q^\dagger X_r^\dagger}]$ since $\underbrace{X_q^\dagger X_r^\dagger} = 0$)

$$= X_q^\dagger X_r^\dagger X_p + \underbrace{X_p X_q^\dagger}\, n[X_r^\dagger]$$

$$- \underbrace{x_p\, x_r^\dagger}\, n[x_q^\dagger]$$

$$= x_q^\dagger x_r^\dagger x_p + \delta_{pq}\, x_r^\dagger$$

$$- \delta_{pr}\, x_q^\dagger$$

Proof of Wick's theorem requires two lemmas.

Lemma 1:

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

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

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

Proof (sketch):

$$M_{m+1} = \underset{\text{difficult}}{X_r^\dagger} \text{ or } \overset{\text{easy}}{X_r}$$

$$n[M_1 \ldots M_m] X_r^\dagger \overset{\text{MUST}}{\underset{\text{PROVE}}{=}} n[M_1 \ldots M_m X_r^\dagger]$$

$$+ \sum_{i=1}^{m} n[M_1 \ldots M_{\bar{i}} \ldots M_m X_r^\dagger]$$

all $M_1, \ldots, M_m$ are annihilators

|| hard

easier

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

$$\Downarrow$$

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

<u>MUST</u>
PROVE

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

proof
by induction
(videos 6, 7)