HOLE-PARTICLE FORMALISM

$$Y_i = X_i^\dagger, \quad Y_i^\dagger = X_i$$

$$Y_a = X_a, \quad Y_a^\dagger = X_a^\dagger$$

1. $$Y_p|\Phi\rangle = 0 \quad \forall p$$

$$(X_p|0\rangle = 0)$$

2. $$\{Y_p, Y_q\} = 0, \quad \{Y_p^\dagger, Y_q^\dagger\} = 0$$

$$\{Y_p, Y_q^\dagger\} = \delta_{pq}$$

$$(\{X_p, X_q\} = 0, \quad \{X_p^\dagger, X_q^\dagger\} = 0, \quad \{X_p, X_q^\dagger\} = \delta_{pq})$$

Normal product relative to the Fermi vacuum state $|\Phi\rangle$:

$$N[M_1 \dots M_m] = (-1)^R \gamma^\dagger_{q_{R_1}} \dots \gamma^\dagger_{q_{R_x}} \gamma_{q_{R_{x+1}}} \dots \gamma_{q_{R_m}}$$

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

$$N[\emptyset] \equiv \mathbb{1}$$

Example:

$$N[\gamma^\dagger_p \gamma_q \gamma^\dagger_r] = -\gamma^\dagger_p \gamma^\dagger_r \gamma_q$$
$$= \gamma^\dagger_r \gamma^\dagger_p \gamma_q$$

Another example:

$$N[X_p^\dagger X_q X_r^\dagger]$$

The answer depends on p, q, and r

Suppose $p, q \in$ occ, $r \in$ unocc.
We obtain $(p=i, q=j, r=a)$,

$$N[X_i^\dagger X_j X_a^\dagger]$$

$$= N[Y_i Y_j^\dagger Y_a^\dagger]$$

$$= Y_j^\dagger Y_a^\dagger Y_i = -Y_a^\dagger Y_j^\dagger Y_i$$

$$= X_j X_a^\dagger X_i^\dagger = -X_a^\dagger X_j X_i^\dagger$$

If we used $n[\ldots]$, we would obtain

$$n[x_i^\dagger x_j x_a^\dagger]$$

$$= x_a^\dagger x_i^\dagger x_j = x_a^\dagger(\delta_{ij} - x_j x_i^\dagger)$$

$$= \delta_{ij}\, x_a^\dagger - x_a^\dagger x_j x_i^\dagger$$

$$\neq N[x_i^\dagger x_j x_a^\dagger] \quad (\text{if } i=j)$$

The N-product depends on the values of p, q, and r (single-particle indices, in general)

Properties of $N[\ldots]$:

(i) $N[M] = M$

(ii) $N[N[M_1 \ldots M_m]]$

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

In particular,

$$N[Y_{q_1}^{+} \ldots Y_{q_x}^{+} Y_{q_{x+1}} \ldots Y_{q_m}]$$

$$= Y_{q_1}^{+} \ldots Y_{q_x}^{+} Y_{q_{x+1}} \ldots Y_{q_m}$$

(iii) $N[M_{R_1} \ldots M_{R_m}]$

$$= (-1)^R N[M_1 \ldots M_m],$$

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

Contractions:

$$\overbrace{M_1 M_2} = M_1 M_2 - N[M_1 M_2]$$

$$\overbrace{\gamma_p \gamma_q} = \gamma_p \gamma_q - N[\gamma_p \gamma_q] = 0$$

✓ $$\overbrace{\gamma_p \gamma_q^\dagger} = \gamma_p \gamma_q^\dagger - N[\gamma_p \gamma_q^\dagger]$$
$$= \gamma_p \gamma_q^\dagger + \gamma_q^\dagger \gamma_p = \delta_{pq}$$

$$\overbrace{\gamma_p^\dagger \gamma_q} = \gamma_p^\dagger \gamma_q - N[\gamma_p^\dagger \gamma_q] = 0$$

$$\overbrace{\gamma_p^\dagger \gamma_q^\dagger} = \gamma_p^\dagger \gamma_q^\dagger - N[\gamma_p^\dagger \gamma_q^\dagger] = 0$$

The only time we obtain a nonzero result for $\overbrace{M_1 M_2}$ is when $M_1 = \gamma_p$ and $M_2 = \gamma_p^\dagger$. In that case, we obtain 1.

$$\left(\underbracket{x_p x_q} = 0, \quad \underbracket{x_p x_q^{\dagger}} = \delta_{pq}, \quad \underbracket{x_p^{\dagger} x_q} = 0, \quad \underbracket{x_p^{\dagger} x_q^{\dagger}} = 0 \right)$$

Normal products with contractions:

$$N[M_1 \dots \overbracket{M_{\mu_1} \dots M_{\nu_1}} \dots \overbracket{M_{\mu_\lambda} \dots M_{\nu_\lambda}} \dots M_m]$$

$$= (-1)^R \, \overbracket{M_{\mu_1} M_{\nu_1}} \dots \overbracket{M_{\mu_\lambda} M_{\nu_\lambda}}$$

$$\times \, N[M_{\kappa_1} \dots M_{\kappa_\rho}]$$

$$R = \begin{pmatrix} 1 & 2 & \dots & (2\lambda-1) & (2\lambda) & (2\lambda+1) & \dots & m \\ \mu_1 & \nu_1 & \dots & \mu_\lambda & \nu_\lambda & \kappa_1 & \dots & \kappa_\rho \end{pmatrix}$$

$$N[\overbracket{M_1 M_2}] \neq N[\overbracket{M_2 M_1}]$$

Examples (see videos)

Remark:

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

$$= - \overbracket{X_p X_r^\dagger}\; \overbracket{X_q X_s^\dagger}\, N[X_t X_u^\dagger]$$

The rest of the answer depends on p, q, r, s, t, u (which can be occupied or not)

We anticipate Wick's theorem as follows:

$$M_1 \cdots M_m = N[M_1 \cdots M_m] + \sum_{\cdots} N[M_1 \cdots M_m]$$

We have two options how to proceed:

① translate all operators into $Y, Y^\dagger$ form or

② learn how to calculate contractions $\sqcap$ using operators in the original $X, X^\dagger$ form

①: Some operators are naturally in the $Y, Y^\dagger$ form; example:

$$|\Phi^{a_1 \ldots a_n}_{i_1 \ldots i_n}\rangle = \prod_{\mu=1}^{n} X^{\dagger}_{a_\mu} X_{i_\mu} |\Phi\rangle$$

$$= \prod_{\mu=1}^{n} Y^{\dagger}_{a_\mu} Y^{\dagger}_{i_\mu} |\Phi\rangle \quad ✓$$

Unfortunately, this is usually not the case.

Example:

$$\hat{Z} = \sum_{p,q} \langle p|\hat{z}|q\rangle X^{\dagger}_{p} X_{q} \quad ✓$$

occ. or unocc. occ. or unocc.

$$= \sum_{i,j} \langle i|\hat{z}|j\rangle Y_i Y^{\dagger}_{j} \quad ✓$$

$$+ \sum_{i,a} \langle i|\hat{z}|a\rangle Y_i Y_a \quad ✓$$

$$+ \sum_{a,i} \langle a|\hat{z}|i\rangle \gamma_a^\dagger \gamma_i^\dagger$$

$$+ \sum_{a,b} \langle a|\hat{z}|b\rangle \gamma_a^\dagger \gamma_b$$

For V, we would get $2^4 = 16$ terms.

Option (1) is not good.
We will rely on option (2).

In order to learn how to determine contractions $\sqcap$ involving X and $X^\dagger$, we introduce step functions χ and π.

$$\chi(p) = \begin{cases} 1 & \text{for } p \in occ \\ 0 & \text{for } p \in unocc \end{cases}$$

$$\bar{\pi}(p) = \begin{cases} 0 & \text{for } p \in occ \\ 1 & \text{for } p \in unocc \end{cases}$$

In other words,

$$\chi(i) = 1, \quad \chi(a) = 0,$$

$$\bar{\pi}(i) = 0, \quad \bar{\pi}(a) = 1.$$

✓ $$\chi(p) + \bar{\pi}(p) = 1 \quad \forall p$$

✓ $$\chi(p)\bar{\pi}(p) = 0$$

$$\chi(p)^2 = \chi(p), \quad \bar{\pi}(p)^2 = \bar{\pi}(p).$$

Let us determine

$$\overline{X_p X_q}, \quad \overline{X_p X_q^\dagger}, \quad \overline{X_p^\dagger X_q}, \quad \text{and} \quad \overline{X_p^\dagger X_q^\dagger}$$

$$\overline{X_p X_q} = [\underbrace{\chi(p) + \pi(p)}_{=1}][\underbrace{\chi(q) + \pi(q)}_{=1}]\overline{X_p X_q}$$

$$= \chi(p)\chi(q)\overline{X_p X_q}$$

$$+ \chi(p)\pi(q)\overline{X_p X_q}$$

$$+ \pi(p)\chi(q)\overline{X_p X_q}$$

$$+ \pi(p)\pi(q)\overline{X_p X_q}$$

$$= \chi(p)\chi(q)\cancel{\overline{Y_p^\dagger Y_q^\dagger}} \to 0$$

$$+ \chi(p)\pi(q)\,\cancel{\overbrace{Y_p^\dagger Y_q}} \to 0$$

$$+ \pi(p)\chi(q)\,\overbrace{Y_p Y_q^\dagger} \longrightarrow \delta_{pq}$$

$$+ \pi(p)\pi(q)\,\cancel{\overbrace{Y_p Y_q}} \to 0$$

$$= \pi(p)\chi(q)\,\delta_{pq} = \pi(p)\chi(p)\,\delta_{pq}$$

$$= 0 \Rightarrow \overbrace{X_p X_q} = 0.$$

Similarly, for other cases.

$$\overbrace{X_p X_q} = 0, \quad \overbrace{X_p X_q^\dagger} = \pi(p)\,\delta_{pq},$$

$$\overbrace{X_p^\dagger X_q} = \chi(p)\,\delta_{pq}, \quad \overbrace{X_p^\dagger X_q^\dagger} = 0$$

Simple explanation, for example

$$\overbrace{X(X^\dagger)}_{\text{must be } Y}\;\underbrace{X(X^\dagger)}_{\text{must be } Y^\dagger}$$

$$\overbrace{X_p Y_q} = 0, \quad \overbrace{X_p Y_q^\dagger} = \pi(p)\,\delta_{pq},$$

$$\overbrace{X_p^\dagger Y_q} = 0, \quad \overbrace{X_p^\dagger Y_q^\dagger} = \chi(p)\,\delta_{pq}$$

Similarly,

$$\overbrace{Y_p X_q} = \chi(p)\,\delta_{pq}, \quad \overbrace{Y_p X_q^\dagger} = \pi(p)\,\delta_{pq},$$

$$\overbrace{Y_p^\dagger X_q} = 0, \quad \overbrace{Y_p^\dagger X_q^\dagger} = 0.$$

We should not forget that

$$\overbrace{Y_p Y_q} = 0, \quad \overbrace{Y_p Y_q^\dagger} = \delta_{pq},$$

$$\overline{\gamma_p^\dagger \gamma_q} = 0, \quad \overline{\gamma_p^\dagger \gamma_q^\dagger} = 0.$$

Wick's theorem (in h-p formalism) (WT)

Motivation:

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

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

$$\langle \Phi_{i_1 \dots i_n}^{a_1 \dots a_n} | X^\dagger \dots X | \Phi_{j_1 \dots j_m}^{b_1 \dots b_m} \rangle$$

$$\Downarrow$$

$$\langle \Phi | M_1 \dots M_m | \Phi \rangle$$

Similarly,

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

$$\Downarrow$$

$$\Downarrow$$

$$M_1 \dots M_m |\Phi\rangle .$$

	Original formalism	Hole-particle formalism
Vacuum state	$\lvert 0\rangle$	$\lvert \Phi\rangle$
Creation and annihilation operators	$X^\dagger, X$	$Y^\dagger, Y$
Normal product	$n[\dots]$	$N[\dots]$
Contractions	$\underline{M_1 M_2}$	$\overline{M_1 M_2}$

Normal product with contractions $\quad n[\ldots] \quad N[\ldots]$

The statement of WT:

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

$$+ \sum_{1 \le \mu < \nu \le m} N[M_1 \ldots M_\mu \ldots M_\nu \ldots M_m]$$

$$+ \sum_{\substack{\mu_1 < \nu_1 \\ \mu_2 < \nu_2 \\ \mu_1 < \mu_2,\ \nu_1 \ne \nu_2}} N[M_1 \ldots M_{\mu_1} \ldots M_{\nu_1} \ldots M_{\mu_2} \ldots M_{\nu_2} \ldots M_m]$$

$$+ \ldots$$

We also have GWT.

Skip contractions of operators from the same N group.
We can restate rules 5–7.

Rule 5 (h-p variant):

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

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

Rule 6 (h-p variant):

$Y|\Phi\rangle = 0$

$\langle \Phi | Y^\dagger = 0$

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

$$= \sum_{f.c.} (-1)^R \, \overline{M_{\mu_1} M_{\nu_1}} \cdots \overline{M_{\mu_m} M_{\nu_m}}$$

$$R = \begin{pmatrix} 1 & 2 & \cdots & (2m-1) & (2m) \\ \mu_1 & \nu_1 & \cdots & \mu_m & \nu_m \end{pmatrix}$$

Rule 7 (h-p variant):

$$M_1 \cdots M_m |\Phi\rangle$$

$$= \sum_{\substack{\text{annihilators } \gamma \\ \text{fully contracted} \\ (a\gamma fc)}} (-1)^R \prod_{\mu_k, \nu_k \in C} \overline{M_{\mu_k} M_{\nu_k}}$$

indices of contracted operators

$$\times \underbrace{\prod_{r \notin C} \gamma_r^{\dagger} |\Phi\rangle}_{\text{Slater determinants}}$$

Examples:

① $\langle \{p_1 \ldots p_N\} | Z | \{p_1 \ldots p_N\} \rangle$

and

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

(a) $\langle \Phi | Z | \Phi \rangle$

(b) $\langle \Phi | V | \Phi \rangle$

(we choose $|\{p_1 \ldots p_N\}\rangle$ to be our $|\Phi\rangle$) ✓

(a) $\langle \Phi | Z | \Phi \rangle$

$$= \sum_{pq} \langle p | \hat{z} | q \rangle \langle \Phi | X_p^\dagger X_q | \Phi \rangle$$

$$\overset{\text{rule 6}}{\underset{\text{f.c.}}{=}} \sum_{p,q} \langle p|\hat{z}|q\rangle \langle \Phi| N[X_p^{\dagger} X_q] |\Phi\rangle$$

$$= \sum_{p,q} \langle p|\hat{z}|q\rangle\, \chi(p)\, \delta_{pq}$$

$$= \sum_{p\in \text{occ}} \langle p|\hat{z}|p\rangle$$

$$= \sum_{i} \langle i|\hat{z}|i\rangle$$

$$\left(\sum_{k=1}^{N} \langle p_k|\hat{z}|p_k\rangle \right)$$

(b) $$\langle \Phi|V|\Phi\rangle = \frac{1}{2} \sum_{ij} \langle ij|\hat{v}|ij\rangle_A$$

② $$\langle \{p_1 p_2 \cdots p_N\}| \underset{\text{or } V}{Z} |\{q_1 p_2 \cdots p_N\}\rangle$$

Choose $|\{p_1 \cdots p_N\}\rangle$ to be $|\Phi\rangle$.

(a) $\langle \Phi | Z | \Phi_i^a \rangle$

(b) $\langle \Phi | V | \Phi_i^a \rangle$

$$|\Phi_i^a\rangle = X_a^\dagger X_i |\Phi\rangle = N[\underset{\uparrow\, Y_a^\dagger}{X_a^\dagger} \underset{\uparrow\, Y_i^\dagger}{X_i}] |\Phi\rangle$$

(a) $\langle \Phi | Z | \Phi_i^a \rangle = \langle i | \hat{z} | a \rangle$

(b) $\langle \Phi | V | \Phi_i^a \rangle$

$$= \frac{1}{2} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle$$

$$\times \langle \Phi | X_p^\dagger X_q^\dagger X_s X_r N[X_a^\dagger X_i] |\Phi\rangle$$

$$\langle \Phi | N[X_p^\dagger X_q^\dagger X_s X_r X_a^\dagger X_i] |\Phi\rangle \checkmark$$

$$+\langle\Phi|N[X_p^\dagger X_q^\dagger X_s X_r X_a^\dagger X_i]|\Phi\rangle \checkmark$$

$$+\langle\Phi|N[X_p^\dagger X_q^\dagger X_s X_r X_a^\dagger X_i]|\Phi\rangle$$

$$+\langle\Phi|N[X_p^\dagger X_q^\dagger X_s X_r X_a^\dagger X_i]|\Phi\rangle$$

$$= -\chi(p)\,\chi(q)^{\nearrow i}\,\bar{\eta}(r)^{\nearrow a}\,\delta_{ps}\,\delta_{qi}\,\delta_{ra} \checkmark$$

$$+\ \chi(p)^{\nearrow i}\,\chi(q)\,\bar{\eta}(r)^{\nearrow a}\,\delta_{pi}\,\delta_{qs}\,\delta_{ra} \checkmark$$

$$+\ \chi(p)\,\chi(q)^{\nearrow i}\,\bar{\eta}(s)^{\nearrow a}\,\delta_{pr}\,\delta_{qi}\,\delta_{sa} \checkmark$$

$$-\ \chi(p)^{\nearrow i}\,\chi(q)\,\bar{\eta}(s)^{\nearrow a}\,\delta_{pi}\,\delta_{qr}\,\delta_{sa} \checkmark$$

$$= \chi(p)\,\delta_{qi}\left(\delta_{pr}\delta_{sa} - \delta_{ps}\delta_{ra}\right)$$

$$+ \chi(q)\,\delta_{pi}\left(\delta_{qs}\delta_{ra} - \delta_{qr}\delta_{sa}\right)$$

$$\langle \Phi | V | \Phi_c^a \rangle = \frac{1}{2} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle$$

$$\times \Big[\chi(p)\,\delta_{qi}\left(\delta_{pr}\delta_{sa} - \delta_{ps}\delta_{ra}\right) + \chi(q)\,\delta_{pi}\left(\delta_{qs}\delta_{ra} - \delta_{qr}\delta_{sa}\right) \Big]$$

$$= \frac{1}{2} \sum_{p \in occ} \Big(\langle pi | \hat{v} | pa \rangle - \langle pi | \hat{v} | ap \rangle \Big)$$

$$+ \frac{1}{2} \sum_{q \in occ} \Big(\langle iq | \hat{v} | aq \rangle - \langle iq | \hat{v} | qa \rangle \Big)$$

$$= \frac{1}{2} \sum_j \langle ji | \hat{v} | ja \rangle_A$$

$$+ \frac{1}{2} \sum_j \langle ij | \hat{v} | aj \rangle_A$$

$$= \sum_j \langle ij | \hat{v} | aj \rangle_A$$

3 $$\langle \underbrace{\{p_1 p_2 p_3 \cdots p_N\}}_{= \langle \Phi |} | V | \underbrace{\{q_1 q_2 p_3 \cdots p_N\}}_{| \Phi_{ij}^{ab} \rangle} \rangle$$

$$\langle \Phi | V | \Phi_{ij}^{ab} \rangle = \langle ij | \hat{v} | ab \rangle_A$$

$$|\Phi_{ij}^{ab}\rangle = N[X_a^{+} X_i X_b^{+} X_j]|\Phi\rangle$$

We do not have to consider $\langle\Phi|Z|\Phi_{ij}^{ab}\rangle$. Here is why:

$$\langle\Phi|Z|\Phi_{ij}^{ab}\rangle = \sum_{pq}\langle p|\hat{z}|q\rangle$$

$$\times \langle\Phi| X_p^{+} X_q N[X_a^{+} X_i X_b^{+} X_j]|\Phi\rangle$$

$= 0$, because we cannot contract 2 operators fully with 4 operators.

Other examples:

(a) $\langle \Phi_i^a | Z | \Phi_j^b \rangle$,

(b) $\langle \Phi_i^a | V | \Phi_j^b \rangle$,

(c) $\langle \Phi_{ij}^{ab} | V | \Phi_{kl}^{cd} \rangle$, etc.

(a) $\langle \Phi_i^a | Z | \Phi_j^b \rangle$

$$= \sum_{pq} \langle p | \hat{z} | q \rangle$$

$$\times \underbrace{\langle \Phi | N[X_i^\dagger X_a]}_{\langle \Phi_i^a |} X_p^\dagger X_q \underbrace{N[X_b^\dagger X_j] | \Phi \rangle}_{| \Phi_j^b \rangle}$$

$$= \sum_{p,q} \langle p | \tfrac{1}{z} | q \rangle$$

$$\times \Big\{ \langle \Phi | N[X_i^\dagger X_a X_p^\dagger X_q X_b^\dagger X_j] | \Phi \rangle$$

$$+ \langle \Phi | N[X_i^\dagger X_a X_p^\dagger X_q X_b^\dagger X_j] | \Phi \rangle$$

$$+ \langle \Phi | N[X_i^\dagger X_a X_p^\dagger X_q X_b^\dagger X_j] | \Phi \rangle \Big\} \checkmark$$

$$= \sum_{p,q} \langle p | \tfrac{1}{z} | q \rangle \Big\{ \delta_{ij} \delta_{pa} \delta_{qb}$$

$$- \delta_{ab}\delta_{pj}\delta_{qi} + \chi(p)\,\delta_{pq}\delta_{ab}\delta_{ij} \Big\}$$

$$\langle \Phi_i^a | Z | \Phi_j^b \rangle = \langle a|\hat{z}|b\rangle \delta_{ij}$$

$$- \langle j|\hat{z}|i\rangle \delta_{ab}$$

$$+ \Big(\sum_{k} \langle k|\hat{z}|k\rangle \Big) \delta_{ab}\delta_{ij}$$

k occ. in $|\Phi\rangle$

$$\sum_k \langle k|\hat{z}|k\rangle = \langle \Phi | Z | \Phi \rangle$$

$$\delta_{ab}\delta_{ij} = \langle \Phi_i^a | \Phi_j^b \rangle$$

If Z was in the normal product form, we would not have to consider the third term.

Z in the normal product form means

$$Z_N = \sum_{pq} \langle p|z|q\rangle N[X_p^+ X_q]$$

It seems to be useful to relate Z to Z_N.

Normal product forms of many-body operators

$$Z = \sum_{p,q} \langle p|\hat{z}|q\rangle X_p^\dagger X_q$$

$$\overset{\text{WT}}{=} \sum_{p,q} \langle p|\hat{z}|q\rangle N[X_p^\dagger X_q]$$

$$+ \sum_{p,q} \langle p|\hat{z}|q\rangle N[\overline{X_p^\dagger X_q}]$$

$$= Z_N + \sum_{p,q} \langle p|\hat{z}|q\rangle \chi(p)\,\delta_{pq}$$

$$= Z_N + \underbrace{\sum_{p\in\text{occ.}} \langle p|\hat{z}|p\rangle}_{\sum_i \langle i|\hat{z}|i\rangle \,=\, \langle\Phi|Z|\Phi\rangle}$$

$$Z = Z_N + \underbrace{\langle \Phi | Z | \Phi \rangle}_{\text{mean-field part}}$$

$$V = \frac{1}{2} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle \times x_p^\dagger x_q^\dagger x_s x_r$$

$$V = \underbrace{V_N}_{\text{no contractions}} + \underbrace{G_N}_{\text{single contractions}} + \underbrace{\langle \Phi | V | \Phi \rangle}_{\text{f.c.}} \checkmark$$

$$V_N = \frac{1}{2} \sum_{pq,rs} \langle pq | \hat{v} | rs \rangle \times N[x_p^\dagger x_q^\dagger x_s x_r]$$

$$= \frac{1}{4} \sum_{pq,r,s} \langle pq|\hat{v}|rs\rangle_A$$

$$\times N[X_p^\dagger X_q^\dagger X_s X_r]$$

$$G_N = \sum_{pq} \langle p|\hat{g}|q\rangle N[X_p^\dagger X_q]$$

$$\langle p|\hat{g}|q\rangle = \sum_{i} \underbrace{\langle pi|\hat{v}|qi\rangle_A}_{\langle pi|\hat{v}|qi\rangle - \langle pi|\hat{v}|iq\rangle}$$

$$\langle \Phi|V|\Phi\rangle = \frac{1}{2} \sum_{ij} \langle ij|\hat{v}|ij\rangle_A$$

In general, we can relate

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

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

with

$\hat{O}_{k,N}$ and $(k-1)$-body, $(k-2)$-body, etc. normal-ordered operators all the way to the $\langle \Phi | \hat{O}_k | \Phi \rangle$ term.

Going back to Z and V...

$$
\begin{aligned}
H &= Z + V \\
&= Z_N + \langle \Phi | Z | \Phi \rangle \\
&\quad + V_N + G_N + \langle \Phi | V | \Phi \rangle \\
&= F_N + V_N + \langle \Phi | H | \Phi \rangle
\end{aligned}
$$

$$F_N = Z_N + G_N$$

mean-field value of energy

$$
\boxed{
\begin{aligned}
H_N &= H - \langle \Phi | H | \Phi \rangle \\
&= F_N + V_N
\end{aligned}
}
$$

correlation effects

$$F_N = \sum_{p,q} \langle p | \hat{f} | q \rangle N[X_p^\dagger X_q]$$

$$\hat{f} = \hat{z} + \hat{g}$$ ← Fock operator

$$\langle p | \hat{f} | q \rangle = \langle p | \hat{z} | q \rangle + \langle p | \hat{g} | q \rangle = \langle p | \hat{z} | q \rangle + \sum_i \langle p i | \hat{v} | q i \rangle_A$$

Going back to matrix elements ...

$$\langle \Phi_i^a | Z_N | \Phi_j^b \rangle$$

$$= \delta_{ij} \langle a | \hat{z} | b \rangle - \delta_{ab} \langle j | \hat{z} | i \rangle$$

How about

$$\langle \Phi_i^a | V | \Phi_j^b \rangle \ ?$$

Use $V = V_N + G_N + \langle \Phi | V | \Phi \rangle$.

$$\langle \Phi_i^a | V | \Phi_j^b \rangle = \langle \Phi_i^a | V_N | \Phi_j^b \rangle$$

$$+ \langle \Phi_i^a | G_N | \Phi_j^b \rangle \checkmark$$

$$+ \underbrace{\langle \Phi | V | \Phi \rangle}_{= \frac{1}{2} \sum_{k,l} \langle kl | \hat{v} | kl \rangle_A} \langle \Phi_i^a | \Phi_j^b \rangle \checkmark$$

$$\langle \Phi_i^a | \Phi_j^b \rangle = \delta_{ij}\,\delta_{ab}$$

$$\left(\langle \Phi_i^a | \Phi_j^b \rangle = \langle \Phi | N[X_i^\dagger X_a X_b^\dagger X_j] | \Phi \rangle \right)$$

$$\langle \Phi_i^a | G_N | \Phi_j^b \rangle$$

$$= \delta_{ij} \langle a | \hat{g} | b \rangle - \delta_{ab} \langle j | \hat{g} | i \rangle$$

$$= \delta_{ij} \sum_k \langle ak | \hat{v} | bk \rangle_A$$

$$- \delta_{ab} \sum_k \langle jk | \hat{v} | ik \rangle_A$$

$$\langle \Phi_i^a | V_N | \Phi_j^b \rangle =$$

$$= \frac{1}{2} \sum_{pqrs} \langle \overset{1}{p}\overset{2}{q} | \hat{v} | \overset{1}{r}\overset{2}{s} \rangle$$

$$\times \langle \Phi | N[X_i^\dagger X_a] \underbrace{N[X_p^\dagger X_q^\dagger X_s X_r]}_{N[X_p^\dagger X_r X_q^\dagger X_s]} N[X_b^\dagger X_j] | \Phi \rangle$$

$$1 \qquad 2$$

$$\ldots = \langle aj | \hat{v} | ib \rangle_A$$

$$\langle \Phi_i^a | V | \Phi_j^b \rangle = \langle aj | \hat{v} | ib \rangle_A$$

$$+ \delta_{ij} \langle a | \hat{g} | b \rangle - \delta_{ab} \langle j | \hat{g} | i \rangle$$

$$+ \delta_{ij} \delta_{ab} \langle \Phi | V | \Phi \rangle$$

One can also redo the previous examples.
Here is one!

$$\langle \Phi | V | \Phi_i^a \rangle = \cancelto{0}{\langle \Phi | V_N | \Phi_i^a \rangle}$$

$$+ \langle \Phi | G_N | \Phi_i^a \rangle$$

$$+ \cancelto{0}{\langle \Phi | V | \Phi \rangle \langle \Phi | \Phi_i^a \rangle}$$

$$\langle \Phi | V_N | \Phi_i^a \rangle = \frac{1}{2} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle$$

$$\times \langle \Phi | N[X_p^\dagger X_q^\dagger X_s X_r] N[X_a^\dagger X_i] | \Phi \rangle$$

$$= 0$$ (can't contract 2 operators with 4)

$$\langle \Phi | G_N | \Phi_i^a \rangle = \sum_{pq} \langle p | g | q \rangle \times \langle \Phi | N[X_p^\dagger X_q] N[X_a^\dagger X_i] | \Phi \rangle$$

$$= \sum_{pq} \langle p | g | q \rangle \times \langle \Phi | N[\underbrace{X_p^\dagger X_q X_a^\dagger X_i}_{\delta_{pi}\,\delta_{qa}}] | \Phi \rangle$$

$$= \langle i | g | a \rangle$$

$$\langle \Phi | V | \Phi_i^a \rangle = \langle i | g | a \rangle = \sum_j \langle ij | v | aj \rangle_A$$

NEXT STOP:

DIAGRAMS