

Wick's Theorem

Wick's Theorem

normal order

normal order

$$a_{p_1}^+ \cdots a_{p_m}^+ a_{q_1} \cdots a_{q_n}$$

normal order

$$a_{p_1}^+ \cdots a_{p_m}^+ a_{q_1} \cdots a_{q_n}$$

↓
vanishing vac expectation
value

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$$:q_1 \cdots q_n: = \sum_{\pi} q_{\pi(1)} \cdots q_{\pi(n)}$$

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$$: q_1 \cdots q_n : = \sum_{\pi} q_{\pi(1)} \cdots q_{\pi(n)}$$

→ where π puts string in
normal order

$$: a_p a_q : = a_p a_q$$

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$$: a_p^\dagger a_q^\dagger : = a_p^\dagger a_q^\dagger$$

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$$: a_p^{\dagger} a_q^{\dagger} : = a_p^{\dagger} a_q^{\dagger}$$

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$$: a_p^\dagger a_q^\dagger : = a_p^\dagger a_q^\dagger$$

$$: a_p^\dagger a_q : = a_p^\dagger a_q$$

$$: a_p a_q^\dagger : = - a_q^\dagger a_p$$

contraction:

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$$\overline{q_1 q_2}$$

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$$\overline{q_1 q_2} \equiv q_1 q_2 - :q_1 q_2:$$

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$$\overline{a_p a_q}$$

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$$\overline{a_p a_q^+} = a_p a_q^+ - (-a_q^+ a_p)$$

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$$\overline{a_p a_q^+} = a_p a_q^+ - (-a_q^+ a_p) = [a_p, a_q^+]_+$$

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$$\begin{aligned} \overline{a_p a_q^+} &= a_p a_q^+ - (-a_q^+ a_p) = [a_p, a_q^+]_+ \\ &= \delta_{pq} \end{aligned}$$

note:

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$$\Rightarrow q_1 q_2 = :q_1 q_2: + \overline{q_1 q_2}$$

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normal-ordered



contraction

normal-ordered with contraction

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$$: q_1 \cdots \overbrace{q_i \cdots q_j} \cdots q_n :$$

normal-ordered with contraction

$$: q_1 \cdots \overbrace{q_i \cdots q_j} \cdots q_n :$$

$$\equiv (-)^{j-i+1} \overbrace{q_i q_j} : q_1 \cdots \cancel{q_i} \cdots \cancel{q_j} \cdots q_n :$$

Wick's theorem:

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$$q_1 q_2 = :q_1 q_2: + \overbrace{q_1 q_2}$$

generalizes to

$$q_1 \cdots q_n = :q_1 \cdots q_n:$$

$$+ \sum :q_1 \cdots \overbrace{q_i \cdots q_j} \cdots q_n:$$

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generalizes to

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$$+ \sum :q_1 \cdots \overbrace{q_i \cdots q_k \cdots q_j} \cdots q_n:$$

Wick's theorem:

$$q_1 q_2 = :q_1 q_2: + \overbrace{q_1 q_2}$$

generalizes to

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$$+ \sum :q_1 \cdots \overbrace{q_i \cdots q_j} \cdots q_n:$$

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+ ...

Wick's theorem:

$$Q = :Q: + :\overline{Q}:$$

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$$Q = :Q: + :\overline{Q}: \downarrow$$

sum of unique
single, double, triple,
etc. contractions

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$$Q = :Q: + :\overline{Q}:$$

Corollary 1.

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$$:Q::Q': = :QQ': + :\overbrace{QQ'}':$$

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Corollary 1.

cross-contractions

$$:Q::Q': = :QQ': + :\overbrace{QQ'}':$$

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Corollary 2.

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Corollary 1.

$$:Q::Q': = :QQ': + :\overbrace{QQ'}:$$

Corollary 2.

$$\langle vac|Q|vac\rangle = :\overline{\overline{Q}}:$$

Wick's Theorem:

$$Q = :Q: + :\overline{Q}:$$

Corollary 1.

$$:Q::Q': = :QQ': + :\overbrace{QQ'}:$$

Corollary 2. complete contractions

$$\langle \text{vac} | Q | \text{vac} \rangle = :\overline{\overline{Q}}:$$

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$$\overline{b_p b_q} = 0$$

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$$\overline{b_p^+ b_q} = 0$$

$$\overline{b_p b_q^+} = \delta_{pq}$$

Φ -normal contraction

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$$\overline{b_p b_q} = 0$$

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$$\overline{b_p^+ b_q} = 0 \rightarrow \overline{a_a^+ a_b} = 0$$

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$$\overline{b_p b_q^+} = \delta_{pq} \rightarrow \overline{a_a a_b^+} = \delta_{ab}$$

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$$\overline{b_p^+ b_q} = 0 \rightarrow \overline{a_a^+ a_b} = 0 \quad \overline{a_i^+ a_j} = 0$$

$$\overline{b_p b_q^+} = \delta_{pq} \rightarrow \overline{a_a a_b^+} = \delta_{ab} \quad \overline{a_i a_j^+} = \delta_{ij}$$

Φ -normal contraction

$$\overline{a_a^+} a_b = 0$$

$$\overline{a_i^+} a_j = 0$$

$$\overline{a_a^+} a_b^+ = \delta_{ab}$$

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$$\overline{q_1 q_2} \equiv q_1 q_2 - :q_1 q_2:$$

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$$\overline{q_1 q_2} \equiv q_1 q_2 - :q_1 q_2:$$

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kills Φ

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kills Φ

$$= \langle \Phi | q_1 q_2 | \Phi \rangle$$

one-hole
density matrix

$$\overline{a_p a_q^\dagger} = \langle \Phi | a_p a_q^\dagger | \Phi \rangle \equiv \eta_{pq}$$

one-hole
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$$\begin{bmatrix} 0 & 0 \\ 0 & \ddots \end{bmatrix}$$

one-hole
density matrix

$$\begin{bmatrix} \textcircled{0} & \textcircled{0} \\ \textcircled{0} & \text{---} \end{bmatrix}$$

$$\overline{a_p a_q^\dagger} = \langle \Phi | a_p a_q^\dagger | \Phi \rangle \equiv \eta_{pq}$$

$$\overline{a_i a_j^\dagger} = 0$$

$$\overline{a_a a_b^\dagger} = \delta_{ab}$$

one-hole
density matrix

$$\begin{bmatrix} \textcircled{0} & \textcircled{0} \\ \textcircled{0} & \text{---} \end{bmatrix}$$

one-particle
density matrix

$$\overline{a_p a_q^\dagger} = \langle \Phi | a_p a_q^\dagger | \Phi \rangle \equiv \eta_{pq}$$

$$\overline{a_i a_j^\dagger} = 0$$

$$\overline{a_a a_b^\dagger} = \delta_{ab}$$

$$\overline{a_p^\dagger a_q} = \langle \Phi | a_p^\dagger a_q | \Phi \rangle \equiv \gamma_{pq}$$

one-hole
density matrix

$$\begin{bmatrix} \circ & \circ \\ \circ & \text{---} \end{bmatrix}$$

$$\overline{a_p a_q^+} = \langle \Phi | a_p a_q^+ | \Phi \rangle \equiv \eta_{pq}$$

$$\overline{a_i a_j^+} = 0$$

$$\overline{a_a a_b^+} = \delta_{ab}$$

one-particle
density matrix

$$\begin{bmatrix} \text{---} & \circ \\ \circ & \circ \end{bmatrix}$$

$$\overline{a_p^+ a_q} = \langle \Phi | a_p^+ a_q | \Phi \rangle \equiv \gamma_{pq}$$

one-hole
density matrix

$$\begin{bmatrix} \textcircled{0} & \textcircled{0} \\ \textcircled{0} & \text{---} \end{bmatrix}$$

$$\overline{a_p a_q^+} = \langle \Phi | a_p a_q^+ | \Phi \rangle \equiv \eta_{pq}$$

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one-particle
density matrix

$$\begin{bmatrix} \text{---} & \textcircled{0} \\ \textcircled{0} & \textcircled{0} \end{bmatrix}$$

$$\overline{a_p^+ a_q} = \langle \Phi | a_p^+ a_q | \Phi \rangle \equiv \gamma_{pq}$$

$$\overline{a_i^+ a_j} = \delta_{ij}$$

$$\overline{a_a^+ a_b} = 0$$

Wick's thm. $Q = :Q: + :\overline{Q}:$

Corollary 1. $:Q::Q': = :QQ': + :\overline{Q}Q':$

Corollary 2. $\langle vac|Q|vac\rangle = :\overline{\overline{Q}}:$

Wick's thm. $Q = :Q: + :\overline{Q}:$

Corollary 1. $:Q::Q': = :QQ': + :\overline{Q}Q':$

Corollary 2. $\langle vac|Q|vac\rangle = :\overline{\overline{Q}}:$

now, contractions are $\overline{a_p^+} a_q = \delta_{pq}$ and $\overline{a_p} a_q^+ = \eta_{pq}$

Examples:

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$$a_p^\dagger a_q$$

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

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Examples:

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

$$\begin{aligned}\langle \Phi | a_p^\dagger a_q | \Phi \rangle &= :\overline{a_p^\dagger} a_q: \\ &= \gamma_{pq}\end{aligned}$$

Examples:

$$a_p^+ a_q^+ a_s a_r$$

Examples:

$$a_p^+ a_q^+ a_s a_r = : a_p^+ a_q^+ a_s a_r :$$

Examples:

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

Examples:

$$a_p^+ a_q^+ a_s a_r =: a_p^+ a_q^+ a_s a_r ::$$

$$+ \overbrace{a_p^+ a_q^+} a_s a_r : + \overbrace{a_p^+ a_q^+ a_s} a_r :$$

Examples:

$$a_p^+ a_q^+ a_s a_r = : a_p^+ a_q^+ a_s a_r :$$

$$+ : \overbrace{a_p^+ a_q^+} a_s a_r : + : \overbrace{a_p^+ a_q^+ a_s} a_r :$$

$$+ : a_p^+ \overbrace{a_q^+} a_s a_r :$$

Examples:

$$a_p^+ a_q^+ a_s a_r =: a_p^+ a_q^+ a_s a_r ::$$

$$+ \overbrace{a_p^+ a_q^+}^{\quad} a_s a_r : + \overbrace{a_p^+ a_q^+ a_s}^{\quad} a_r :$$

$$+ \overbrace{a_p^+}^{\quad} \overbrace{a_q^+}^{\quad} a_s a_r : + \overbrace{a_p^+ a_q^+}^{\quad} a_s a_r :$$

Examples:

$$a_p^+ a_q^+ a_s a_r =: a_p^+ a_q^+ a_s a_r :$$

$$+ \overbrace{a_p^+ a_q^+}^+ a_s a_r : + \overbrace{a_p^+ a_q^+ a_s}^+ a_r :$$

$$+ \overbrace{a_p^+}^+ a_q^+ a_s a_r : + \overbrace{a_p^+ a_q^+}^+ a_s a_r :$$

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Examples:

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$$\langle \Phi | a_p^+ a_q^+ a_s a_r | \Phi \rangle = : \overbrace{a_p^+ \overbrace{a_q^+} a_s} a_r : + : \overbrace{a_p^+ \overbrace{a_q^+} a_s} a_r :$$

Examples:

$$a_p^+ a_q^+ a_s a_r = : a_p^+ a_q^+ a_s a_r :$$

$$+ : \overbrace{a_p^+ a_q^+} a_s a_r : + : \overbrace{a_p^+ a_q^+} a_s a_r :$$

$$+ : a_p^+ \overbrace{a_q^+} a_s a_r : + : a_p^+ \overbrace{a_q^+} a_s a_r :$$

$$+ : \overbrace{a_p^+ \overbrace{a_q^+} a_s} a_r : + : \overbrace{a_p^+ \overbrace{a_q^+} a_s} a_r :$$

$$\begin{aligned} \langle \Phi | a_p^+ a_q^+ a_s a_r | \Phi \rangle &= : \overbrace{a_p^+ \overbrace{a_q^+} a_s} a_r : + : \overbrace{a_p^+ \overbrace{a_q^+} a_s} a_r : \\ &= \gamma_{pr} \gamma_{qs} - \gamma_{ps} \gamma_{qr} \end{aligned}$$

$$\hat{H}_e = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\hat{H}_e = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} \langle pq | rs \rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\langle \Phi | \hat{H}_e | \Phi \rangle = \sum_{pq} h_{pq} \langle \Phi | a_p^\dagger a_q | \Phi \rangle + \frac{1}{2} \sum_{pqrs} \langle pq | rs \rangle \langle \Phi | a_p^\dagger a_q^\dagger a_s a_r | \Phi \rangle$$

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$$= \sum_{pq} h_{pq} \gamma_{pq} + \frac{1}{2} \sum_{pqrs} \langle pq | rs \rangle (\gamma_{pr} \gamma_{qs} - \gamma_{ps} \gamma_{qr})$$

$$\hat{H}_e = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} \langle pq | rs \rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\langle \Phi | \hat{H}_e | \Phi \rangle = \sum_{pq} h_{pq} \langle \Phi | a_p^\dagger a_q | \Phi \rangle + \frac{1}{2} \sum_{pqrs} \langle pq | rs \rangle \langle \Phi | a_p^\dagger a_q^\dagger a_s a_r | \Phi \rangle$$

$$= \sum_{pq} h_{pq} \gamma_{pq} + \frac{1}{2} \sum_{pqrs} \langle pq | rs \rangle (\gamma_{pr} \gamma_{qs} - \gamma_{ps} \gamma_{qr})$$

$$= \sum_i h_{ii} + \frac{1}{2} \sum_{i\bar{j}} \langle ij || i\bar{j} \rangle$$

Now you try!

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We can make life simpler by expanding
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We can make life simpler by expanding H_e in terms of \mathbb{I} -normal ops:

$$H_e = \sum_{pq} h_{pq} (:a_p^\dagger a_q: + :a_p^\dagger a_q:) \\ + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle a_p^\dagger a_q^\dagger a_s a_r$$

We can make life simpler by expanding H_e in terms of \mathbb{I} -normal ops:

$$\begin{aligned}
 H_e = & \sum_{pq} h_{pq} (:a_p^\dagger a_q: + : \overline{a_p^\dagger} a_q :) \\
 & + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle (:a_p^\dagger a_q^\dagger a_s a_r: + : \overline{a_p^\dagger} \overline{a_q^\dagger} a_s a_r: + : \overline{a_p^\dagger} a_q^\dagger a_s a_r: \\
 & + : a_p^\dagger \overline{a_q^\dagger} a_s a_r: + : a_p^\dagger \overline{a_q^\dagger} a_s a_r: + : \overline{a_p^\dagger} \overline{a_q^\dagger} a_s a_r: \\
 & + : \overline{a_p^\dagger} \overline{a_q^\dagger} a_s a_r:)
 \end{aligned}$$

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 H_e = & \sum_{pq} h_{pq} (:a_p^\dagger a_q: + : \overline{a_p^\dagger} a_q:) \\
 & + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle (:a_p^\dagger a_q^\dagger a_s a_r: + : \overline{a_p^\dagger} \overline{a_q^\dagger} a_s a_r: + : \overline{a_p^\dagger} a_q^\dagger a_s a_r: \\
 & + : a_p^\dagger \overline{a_q^\dagger} a_s a_r: + : a_p^\dagger \overline{a_q^\dagger} a_s a_r: + : \overline{a_p^\dagger} \overline{a_q^\dagger} a_s a_r: \\
 & + : \overline{a_p^\dagger} \overline{a_q^\dagger} a_s a_r:) \\
 = &
 \end{aligned}$$

We can make life simpler by expanding H_e in terms of \mathbb{I} -normal ops:

$$\begin{aligned}
 H_e &= \sum_{pq} h_{pq} (:a_p^\dagger a_q: + : \overline{a_p^\dagger} a_q:) \\
 &+ \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle (:a_p^\dagger a_q^\dagger a_s a_r: + : \overline{a_p^\dagger} a_q^\dagger a_s a_r: + : \overline{a_p^\dagger} a_q^\dagger a_s a_r: \\
 &\quad + : a_p^\dagger \overline{a_q^\dagger} a_s a_r: + : a_p^\dagger \overline{a_q^\dagger} a_s a_r: + : \overline{a_p^\dagger} \overline{a_q^\dagger} a_s a_r: \\
 &\quad + : \overline{a_p^\dagger} \overline{a_q^\dagger} a_s a_r:) \\
 &= E_0
 \end{aligned}$$

We can make life simpler by expanding H_e in terms of \mathbb{I} -normal ops:

$$\begin{aligned}
 H_e &= \sum_{pq} h_{pq} (:a_p^\dagger a_q: + :a_p^\dagger a_q:) \\
 &+ \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle (:a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: \\
 &\quad + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: \\
 &\quad + :a_p^\dagger a_q^\dagger a_s a_r:) \\
 &= E_0 + \sum_{pq} f_{pq} :a_p^\dagger a_q:
 \end{aligned}$$

We can make life simpler by expanding H_e in terms of \mathbb{I} -normal ops:

$$\begin{aligned}
 H_e &= \sum_{pq} h_{pq} (:\overset{\text{purple}}{a_p^\dagger} \overset{\text{purple}}{a_q}: + :\overset{\text{green}}{\overbrace{a_p^\dagger}^{\text{green}}} \overset{\text{green}}{a_q}:) \\
 &\quad + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle (:\overset{\text{red}}{a_p^\dagger} \overset{\text{red}}{a_q^\dagger} \overset{\text{red}}{a_s} \overset{\text{red}}{a_r}: + :\overset{\text{purple}}{\overbrace{a_p^\dagger a_q^\dagger}^{\text{purple}}} \overset{\text{purple}}{a_s} \overset{\text{purple}}{a_r}: + :\overset{\text{purple}}{\overbrace{a_p^\dagger}^{\text{purple}}} \overset{\text{purple}}{\overbrace{a_q^\dagger}^{\text{purple}}} \overset{\text{purple}}{a_s} \overset{\text{purple}}{a_r}: \\
 &\quad + :\overset{\text{purple}}{a_p^\dagger} \overset{\text{purple}}{\overbrace{a_q^\dagger}^{\text{purple}}} \overset{\text{purple}}{a_s} \overset{\text{purple}}{a_r}: + :\overset{\text{purple}}{a_p^\dagger} \overset{\text{purple}}{\overbrace{a_q^\dagger}^{\text{purple}}} \overset{\text{purple}}{a_s} \overset{\text{purple}}{a_r}: + :\overset{\text{green}}{\overbrace{a_p^\dagger}^{\text{green}}} \overset{\text{green}}{\overbrace{a_q^\dagger}^{\text{green}}} \overset{\text{green}}{\overbrace{a_s}^{\text{green}}} \overset{\text{green}}{\overbrace{a_r}^{\text{green}}}: \\
 &\quad + :\overset{\text{green}}{\overbrace{a_p^\dagger}^{\text{green}}} \overset{\text{green}}{\overbrace{a_q^\dagger}^{\text{green}}} \overset{\text{green}}{\overbrace{a_s}^{\text{green}}} \overset{\text{green}}{\overbrace{a_r}^{\text{green}}}:) \\
 &= E_0 + \sum_{pq} f_{pq} :\overset{\text{purple}}{a_p^\dagger} \overset{\text{purple}}{a_q}: + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle :\overset{\text{red}}{a_p^\dagger} \overset{\text{red}}{a_q^\dagger} \overset{\text{red}}{a_s} \overset{\text{red}}{a_r}:
 \end{aligned}$$

We can make life simpler by expanding H_e in terms of \mathbb{E} -normal ops:

$$\begin{aligned}
 H_e &= \sum_{pq} h_{pq} (:a_p^\dagger a_q: + :a_p^\dagger a_q:) \\
 &\quad + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle (:a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: \\
 &\quad + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: \\
 &\quad + :a_p^\dagger a_q^\dagger a_s a_r:) \\
 &= E_0 + \sum_{pq} f_{pq} :a_p^\dagger a_q: + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle :a_p^\dagger a_q^\dagger a_s a_r: \\
 &\quad \rightarrow \sum_i h_{ii} + \frac{1}{2} \sum_{ij} \langle ij || ij \rangle
 \end{aligned}$$

We can make life simpler by expanding H_e in terms of \mathbb{E} -normal ops:

$$\begin{aligned}
 H_e &= \sum_{pq} h_{pq} (:a_p^\dagger a_q: + :a_p^\dagger a_q:) \\
 &\quad + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle (:a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: \\
 &\quad + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: + :a_p^\dagger a_q^\dagger a_s a_r: \\
 &\quad + :a_p^\dagger a_q^\dagger a_s a_r:) \\
 &= E_0 + \sum_{pq} f_{pq} :a_p^\dagger a_q: + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle :a_p^\dagger a_q^\dagger a_s a_r: \\
 &\quad \xrightarrow{\quad} \sum_i h_{ii} + \frac{1}{2} \sum_{ij} \langle ij || ij \rangle \quad h_{pq} + \sum_i \langle pi || qi \rangle
 \end{aligned}$$

Compare the work for $\langle \Phi | H_e | \Phi \rangle$:

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$$\begin{aligned} \langle \Phi | H_e | \Phi \rangle = E_0 &+ \sum_{pq} f_{pq} \langle \Phi | :a_p^\dagger a_q: | \Phi \rangle \\ &+ \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \langle \Phi | :a_p^\dagger a_q^\dagger a_s a_r: | \Phi \rangle \end{aligned}$$

Compare the work for $\langle \Phi | H_e | \Phi \rangle$:

$$\begin{aligned} \langle \Phi | H_e | \Phi \rangle = E_0 &+ \sum_{pq} f_{pq} \langle \Phi | : \cancel{a_p^\dagger a_q} : | \Phi \rangle \\ &+ \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \langle \Phi | : \cancel{a_p^\dagger a_q^\dagger a_s a_r} : | \Phi \rangle \end{aligned}$$

Compare the work for $\langle \Phi | H_e | \Phi \rangle$:

$$\begin{aligned} \langle \Phi | H_e | \Phi \rangle &= E_0 + \sum_{pq} f_{pq} \langle \Phi | : \cancel{a_p^\dagger a_q} : | \Phi \rangle \\ &\quad + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \langle \Phi | : \cancel{a_p^\dagger a_q^\dagger a_s a_r} : | \Phi \rangle \\ &= E_0 \end{aligned}$$

Compare the work for $\langle \Phi | H_e | \Phi \rangle$:

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Compare the work for $\langle \Phi | H_e | \Phi \rangle$:

$$\begin{aligned} \langle \Phi | H_e | \Phi \rangle &= E_0 + \sum_{pq} f_{pq} \langle \Phi | : \cancel{a_p^\dagger a_q} : | \Phi \rangle \\ &\quad + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \langle \Phi | : \cancel{a_p^\dagger a_q^\dagger a_s a_r} : | \Phi \rangle \\ &= E_0 = \sum_i h_{ii} + \frac{1}{2} \sum_{ij} \langle ij || ij \rangle \end{aligned}$$

Now you try!

1. $\langle \Phi | H_e | \Phi_i^a \rangle$

2. $\langle \Phi | H_e | \Phi_{ij}^{ab} \rangle$

3. $\langle \Phi_i^a | H_e | \Phi_j^b \rangle$

the end.