$$|\Psi_0\rangle = \Omega|\Phi_0\rangle$$

$$\Omega = P + Q_{k_0} W P$$

$$= P + \sum_{n=0}^{\infty} (R^{(0)} W')^n R^{(0)} W P$$

$$k_0 = \varkappa_0 + \langle\Phi_0|\tau|\Phi_0\rangle$$

$$\tau = PW\Omega$$

$$= PWP + \sum_{n=0}^{\infty} PW (R^{(0)} W')^n R^{(0)} W P$$

$$W' = W - (k_0 - \varkappa_0)$$

$$k_0 = \varkappa_0 + \sum_{m=1}^{\infty} k_0^{(m)}$$

$$W' = W - \sum_{m=1}^{\infty} K_0^{(m)}$$

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{n=1}^{\infty} |\Psi_0^{(n)}\rangle$$

0th order

$$|\Psi_0\rangle = |\Phi_0\rangle$$

at least 1st order

$$+ \sum_{n=0}^{\infty} (R^{(0)} W')^n R^{(0)} W |\Phi_0\rangle$$

0th order   1st order

$$K_0 = E_0 + \langle \Phi_0 | W | \Phi_0 \rangle$$

$$+ \sum_{n=0}^{\infty} \langle \Phi_0 | W (R^{(0)} W')^n R^{(0)} W | \Phi_0 \rangle$$

at least 2nd order

$$W' = W - \big(\overbrace{K_0 - E_0}^{\sum_{m=1}^{\infty} K_0^{(m)}}\big)$$

at least 1st order

0th order:

$$|\Psi_0^{(0)}\rangle = |\Phi_0\rangle \qquad (\Omega^{(0)} = P)$$

$$k_0^{(0)} = \varkappa_0 \qquad (\tau^{(0)} = 0)$$

1st order:

$$|\Psi_0^{(1)}\rangle = R^{(0)} W |\Phi_0\rangle$$

$$k_0^{(1)} = \langle \Phi_0 | W | \Phi_0 \rangle$$

$$(\Omega^{(1)} = R^{(0)} W P, \ \tau^{(1)} = PWP)$$

2nd order:

$$|\Psi_0^{(2)}\rangle = R^{(0)}\overset{n=1}{(W-k_0^{(1)})}R^{(0)}W|\Phi_0\rangle$$

$$= (R^{(0)}W)^2|\Phi_0\rangle$$

$$-\langle\Phi_0|W|\Phi_0\rangle R^{(0)2}W|\Phi_0\rangle$$

$$k_0^{(2)} = \langle\Phi_0|WR^{(0)}W|\Phi_0\rangle$$

$n=0$

$$\left(\Omega^{(2)} = R^{(0)}(W-k_0^{(1)})R^{(0)}WP,\quad \tau^{(2)} = PWR^{(0)}WP\right)$$

3rd order:

$$|\Psi_0^{(3)}\rangle = \left[R^{(0)}\left(W - \overset{n=2}{\downarrow}\, k_0^{(1)}\right)\right]^2 R^{(0)} W |\Phi_0\rangle$$

$$- k_0^{(2)} R^{(0)2} W |\Phi_0\rangle \leftarrow n=1$$

$$= \left(R^{(0)} W\right)^3 |\Phi_0\rangle$$

$$- \langle\Phi_0|W|\Phi_0\rangle \left(R^{(0)2} W R^{(0)} W |\Phi_0\rangle\right.$$

$$\left. + R^{(0)} W R^{(0)2} W |\Phi_0\rangle\right)$$

$$+ \langle\Phi_0|W|\Phi_0\rangle^2 R^{(0)3} W |\Phi_0\rangle$$

$$- \langle\Phi_0|W R^{(0)} W|\Phi_0\rangle R^{(0)2} W |\Phi_0\rangle$$

$$k_0^{(3)} = \langle \Phi_0 | W R^{(0)} (W - k_0^{(1)}) R^{(0)} W | \Phi_0 \rangle$$

n=1

$$= \langle \Phi_0 | W R^{(0)} W R^{(0)} W | \Phi_0 \rangle$$

$$- \langle \Phi_0 | W | \Phi_0 \rangle \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle$$

4th order: n=2

$$k_0^{(4)} = \langle \Phi_0 | W [R^{(0)} (W - k_0^{(1)})]^2 R^{(0)} W | \Phi_0 \rangle$$

$$- k_0^{(2)} \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle$$

n=1

$$= \langle \Phi_0 | W R^{(0)} W R^{(0)} W R^{(0)} W | \Phi_0 \rangle$$

$$- \langle \Phi_0 | W | \Phi_0 \rangle \Big(\langle \Phi_0 | W R^{(0)2} W R^{(0)} W | \Phi_0 \rangle$$

$$+ \langle \Phi_0 | W R^{(0)} W R^{(0)2} W | \Phi_0 \rangle \Big)$$

$$+ \langle \Phi_0 | W | \Phi_0 \rangle^2 \langle \Phi_0 | W R^{(0)3} W | \Phi_0 \rangle$$

$$- \langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle$$

$$| \Psi_0^{(n)} \rangle = \left(R^{(0)} W \right)^n | \Phi_0 \rangle$$

+ renormalization terms

$$k_0^{(n+1)} = \langle \Phi_0 | W (R^{(0)} W)^n | \Phi_0 \rangle$$

+ renormalization terms

$$k_0^{(n+1)} = \langle \Phi_0 | W | \Psi_0^{(n)} \rangle$$

Explanation:

$$\tau^{(n+1)} = P W \Omega^{(n)}$$

$$k_0^{(n+1)} = \langle \Phi_0 | \tau^{(n+1)} | \Phi_0 \rangle$$

$$= \langle \Phi_0 | W \underbrace{\Omega^{(n)} | \Phi_0 \rangle}_{| \Psi_0^{(n)} \rangle}$$

We can obtain more explicit formulas by using

$$R^{(0)} = \sum_{n \neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0 - \mathcal{E}_n}$$

Proof:

$$R^{(0)}|\Phi\rangle = |\tilde{\Phi}\rangle \quad \checkmark$$

$$|\tilde{\Phi}\rangle = \sum_n c_n |\Phi_n\rangle,$$

$$c_n = \langle\Phi_n|\tilde{\Phi}\rangle \quad \checkmark$$

$$|\tilde{\Phi}\rangle = (P+Q)|\tilde{\Phi}\rangle$$

$$= \underbrace{PR^{(0)}}_{=0}|\Phi\rangle + QR^{(0)}|\Phi\rangle$$

$$= \sum_{n\neq 0} |\Phi_n\rangle\langle\Phi_n|R^{(0)}|\Phi\rangle$$

$$c_0 = 0, \quad c_n = \langle\Phi_n|R^{(0)}|\Phi\rangle$$

$$Q|\tilde{\Phi}\rangle = |\tilde{\Phi}\rangle$$

$$Q(\varepsilon_0 - K_0) / \; R^{(0)}|\Psi\rangle = |\Psi\rangle$$

$$\underline{Q(\varepsilon_0 - K_0) R^{(0)}|\Psi\rangle} = Q(\varepsilon_0 - K_0)|\Psi\rangle$$

$$Q$$

$$\langle\Phi_n|K_0 = \varepsilon_n\langle\Phi_n|$$

$$Q|\Psi\rangle = \sum_{n\neq 0} |\Phi_n\rangle\langle\Phi_n|(\varepsilon_0 - K_0)|\Psi\rangle$$

$$= \sum_{n\neq 0} (\varepsilon_0 - \varepsilon_n)|\Phi_n\rangle \underbrace{\langle\Phi_n|\Psi\rangle}_{= c_n}$$

$$\sum_{n\neq 0} |\Phi_n\rangle\langle\Phi_n|\Phi\rangle$$

$$= \sum_{n\neq 0} (\varepsilon_0-\varepsilon_n)\, c_n\, |\Phi_n\rangle$$

$$\langle\Phi_n|\Phi\rangle = c_n(\varepsilon_0-\varepsilon_n)$$

$$c_n = \frac{\langle\Phi_n|\Phi\rangle}{\varepsilon_0-\varepsilon_n}$$

$$R^{(0)}|\Phi\rangle = |\tilde{\Phi}\rangle = \sum_{n\neq 0} c_n |\Phi_n\rangle$$

$$= \sum_{n\neq 0} \frac{\langle\Phi_n|\Phi\rangle}{\varepsilon_0-\varepsilon_n} |\Phi_n\rangle$$

$$R^{(0)}|\Phi\rangle = \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|\Phi\rangle}{\mathcal{E}_0-\mathcal{E}_n}$$

$$R^{(0)} = \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0-\mathcal{E}_n}$$

$\therefore$

Examples:

$$|\Psi_0^{(1)}\rangle = \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|W|\Phi\rangle}{\mathcal{E}_0-\mathcal{E}_n}$$

$$|\Psi_0^{(2)}\rangle = \sum_{m\neq 0} \frac{|\Phi_m\rangle\langle\Phi_m|}{\mathcal{E}_0-\mathcal{E}_m} W$$

$$\times \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0-\mathcal{E}_n} W |\Phi_0\rangle$$

$$- \langle\Phi_0|W|\Phi_0\rangle \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{(\mathcal{E}_0-\mathcal{E}_n)^2}$$

$$\times W |\Phi_0\rangle$$

We used:

$$[R^{(0)}]^k = \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{(\mathcal{E}_0-\mathcal{E}_n)^k}$$

$$|\Psi_0^{(2)}\rangle =$$

$$= \sum_{m,n\neq 0} \frac{|\Phi_m\rangle\langle\Phi_m|W|\Phi_n\rangle\langle\Phi_n|W|\Phi_0\rangle}{(\mathcal{E}_0-\mathcal{E}_m)(\mathcal{E}_0-\mathcal{E}_n)}$$

$$- \langle\Phi_0|W|\Phi_0\rangle \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|W|\Phi_0\rangle}{(\mathcal{E}_0-\mathcal{E}_n)^2}$$

$$K_0^{(2)} = \langle\Phi_0|W \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0-\mathcal{E}_n}$$

$$\times W|\Phi_0\rangle$$

$$= \sum_{n\neq 0} \frac{\langle\Phi_0|W|\Phi_n\rangle\langle\Phi_n|W|\Phi_0\rangle}{\mathcal{E}_0-\mathcal{E}_n}$$

BRACKETING TECHNIQUE (Huby, 1961)

principal term

$$|\Psi_0^{(n)}\rangle = (R^{(0)}W)^n|\Phi_0\rangle$$

$+$ renormalization terms

principal term

$$K_0^{(n+1)} = \langle\Phi_0|W(R^{(0)}W)^n|\Phi_0\rangle$$

$+$ renormalization terms

$(n=0, 1, \ldots)$

$$\langle \Phi_0 | \ldots | \Phi_0 \rangle \Rightarrow \langle \ldots \rangle$$

$$\langle \Phi_0 | W | \Phi_0 \rangle = \langle W \rangle$$

$$\langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle$$

$$= \langle W R^{(0)} W \rangle, \text{ etc.}$$

$$k_0^{(1)} = \langle W \rangle,$$

$$k_0^{(2)} = \langle W R^{(0)} W \rangle,$$

$$k_0^{(3)} = \langle W R^{(0)} W R^{(0)} W \rangle$$

$$- \langle W \rangle \langle W R^{(0)2} W \rangle,$$

$$
\begin{aligned}
K_0^{(4)} = {} & \langle W R^{(0)} W R^{(0)} W R^{(0)} W \rangle \\
& - \langle W \rangle \left[\langle W R^{(0)2} W R^{(0)} W \rangle \right. \\
& \left. + \langle W R^{(0)} W R^{(0)2} W \rangle \right] \\
& + \langle W \rangle^2 \langle W R^{(0)3} W \rangle \\
& - \langle W R^{(0)} W \rangle \langle W R^{(0)2} W \rangle ,
\end{aligned}
$$

etc.

$$K_0^{(n+1)} = \langle W (R^{(0)} W)^n \rangle$$

$$+ \text{ renormalization terms}$$

$$(n \geq 0)$$

To obtain renormalization terms, we insert pairs of brackets, $\langle \ldots \rangle$, such that

- they are non-straddling,
- they cannot touch each other,

- the leftmost and rightmost W cannot be bracketed,
- each bracket pair must have W on each side,

For a given expression with r bracket pairs, we assign a sign factor $(-1)^r$.

Example: $K_0^{(3)}$

Principal term

$$\langle W R^{(0)} W R^{(0)} W \rangle \quad \checkmark$$

Let us try to insert bracket pairs into the principal term (without any reference to Huby's rules)

$$\langle \langle W \rangle R^{(0)} W R^{(0)} W \rangle \to 0$$

$$= \langle W \rangle \underbrace{\langle R^{(0)}}_{\langle \Phi_0 | R^{(0)} = 0} W R^{(0)} W \rangle$$

$$\cancel{\langle W \langle R^{(0)} \rangle W R^{(0)} W \rangle} \to 0$$

$$= \langle R^{(0)} \rangle \langle W^2 R^{(0)} W \rangle$$

$$\langle \Phi | R^{(0)} | \Phi \rangle = 0$$

$$\boxed{\begin{aligned} &\langle W R^{(0)} \langle W \rangle R^{(0)} W \rangle \\ &= \langle W \rangle \langle W R^{(0)2} W \rangle \quad \boxed{r=1} \end{aligned}} \quad \checkmark$$

$$\cancel{\langle W R^{(0)} W \langle R^{(0)} \rangle W \rangle} \to 0$$

$$= \underbrace{\langle R^{(0)} \rangle}_{0} \langle W R^{(0)} W^2 \rangle$$

$$\cancel{\langle W R^{(0)} W R^{(0)} \langle W \rangle \rangle} \to 0$$

$$= \langle W \rangle \langle W R^{(0)} W \underbrace{R^{(0)} \rangle}_{R^{(0)}|\Phi_0\rangle = 0}$$

$$k_0^{(3)} = \langle W (R^{(0)} W)^2 \rangle$$

$$- \langle W \rangle \langle W R^{(0)2} W \rangle$$

Why can't brackets touch?

$$\langle \dots \langle W \dots W \underbrace{\rangle \langle R^{(0)}}_{\langle \Phi_0 | R^{(0)} = 0} \dots W \rangle \dots \rangle$$

$$\langle \dots \langle W \dots \underbrace{R^{(0)} \rangle}_{R^{(0)} | \Phi_0 \rangle = 0} \langle W \dots W \rangle \dots \rangle$$

Why can't we allow bracketing of the leftmost and rightmost Ws?

$$\langle \langle W \ldots W \rangle R^{(0)} \ldots \rangle$$

$$\langle \Phi_0 | R^{(0)} = 0$$

$$\langle \ldots R^{(0)} \langle W \ldots W \rangle \rangle$$

$$R^{(0)} | \Phi_0 \rangle = 0$$

etc.

Another example: $K_0^{(4)}$

Principal term

$$\langle W R^{(0)} W R^{(0)} W R^{(0)} W \rangle$$

Renormalization terms

$$\langle W R^{(0)} \langle W \rangle R^{(0)} W R^{(0)} W \rangle \checkmark$$

$r=1, -$

$$\langle W R^{(0)} W R^{(0)} \langle W \rangle R^{(0)} W \rangle \checkmark$$

$r=1, -$

$$\langle W R^{(0)} \langle W \rangle R^{(0)} \langle W \rangle R^{(0)} W \rangle$$

$r = 2, +$

$$\langle W R^{(0)} \langle W R^{(0)} W \rangle R^{(0)} W \rangle$$

$r = 1, -$

$$k_0^{(4)} = \langle W (R^{(0)} W)^3 \rangle$$

$$- \langle W \rangle \langle W R^{(0)2} W R^{(0)} W \rangle$$

$$- \langle W \rangle \langle W R^{(0)} W R^{(0)2} W \rangle$$

$$+\langle W\rangle^2\langle WR^{(0)3}W\rangle$$

$$-\langle WR^{(0)}W\rangle\langle WR^{(0)2}W\rangle$$

Remember:

You are allowed to place brackets inside other brackets as long as you follow Huby('s) rules.

What about wave function corrections?

Rules are similar:

- brackets are non-straddling,
- they cannot touch each other,
- the rightmost W cannot be bracketed,
- each bracket pair must have W on each side.

For a given expression with r bracket pairs, we assign a sign factor $(-1)^r$.

Examples:

$$|\Psi_0^{(2)}\rangle = R^{(0)} W R^{(0)} W |\Phi_0\rangle - R^{(0)} \langle W \rangle R^{(0)} W |\Phi_0\rangle$$

$r=1$

$$= \left(R^{(0)} W\right)^2 |\Phi_0\rangle - \langle W \rangle R^{(0)2} W |\Phi_0\rangle$$

$$|\Psi_0^{(3)}\rangle = R^{(0)} W R^{(0)} W R^{(0)} W |\Phi_0\rangle$$

$$- \; R^{(0)} \langle W \rangle R^{(0)} W R^{(0)} W |\Phi_0\rangle$$

$r=1$

$$- \; R^{(0)} W R^{(0)} \langle W \rangle R^{(0)} W |\Phi_0\rangle$$

$r=1$

$$+ \; R^{(0)} \langle W \rangle R^{(0)} \langle W \rangle R^{(0)} W |\Phi_0\rangle$$

$r=2$

$$- \; R^{(0)} \langle W R^{(0)} W \rangle R^{(0)} W |\Phi_0\rangle$$

$r=1$

$$
\begin{aligned}
|\Psi_0^{(3)}\rangle &= (R^{(0)}W)^3|\Phi_0\rangle \\
&- \langle W\rangle\left[R^{(0)2}WR^{(0)}W|\Phi_0\rangle\right. \\
&\left.+ R^{(0)}WR^{(0)2}W|\Phi_0\rangle\right] \\
&+ \langle W\rangle^2 R^{(0)3}W|\Phi_0\rangle \\
&- \langle WR^{(0)}W\rangle R^{(0)2}W|\Phi_0\rangle
\end{aligned}
$$

BACK TO MBPT

$$H_N|\Psi_0\rangle = \Delta E_0|\Psi_0\rangle$$

$$H_N = H - \langle\Phi_0|H|\Phi_0\rangle$$

Fermi vacuum

$$|\Phi_0\rangle = |\Psi^{(0)}_0\rangle$$

unperturbed IPM state

$$\Delta E_0 = E_0 - \langle\Phi_0|H|\Phi_0\rangle$$

$$H_N = H - \langle H\rangle$$

$$\Delta E_0 = E_0 - \langle H\rangle$$

$$|\Phi_0\rangle = |\{p_1 \dots p_N\}\rangle$$

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

$$= \prod_{r=1}^{N} X^\dagger_{p_r} |0\rangle$$

We must write H_N as

$$K = H_N = K_0 + W,$$

perturbation

unperturbed Hamiltonian

such that

$$K_0 |\Phi_0\rangle = \varepsilon_0 |\Phi_0\rangle$$

and we can easily determine all eigenstates of K_0,

$$K_0|\Phi_n\rangle = \varepsilon_n|\Phi_n\rangle.$$

W will be defined as

$$W = K - K_0,$$

so that

$$\sum_{n=0}^{\infty} |\Psi_0^{(n)}\rangle = |\Psi_0\rangle$$

and

$$\sum_{n=0}^{\infty} \Delta E_0^{(n)} = \Delta E_0.$$

DEFINITIONS OF $|\Phi\rangle$ AND K_0

$$H = Z + V$$

$$Z = \sum_{rs} \langle r|\hat{z}|s\rangle X_r^\dagger X_s$$

$$V = \frac{1}{2}\sum_{rstu} \langle rs|\hat{v}|tu\rangle$$

$$\times X_r^\dagger X_s^\dagger X_u X_t$$

We will not use Z as an unperturbed operator.

Instead, we will define

$$H_0 = Z + U,$$

where

$$U = \sum_{r,s} \langle r|\hat{u}|s\rangle X_r^\dagger X_s$$

is a one-body operator that can be regarded as an approximation to V, $U \approx V$.

In first quantization,

$$U = \sum_{i=1}^{N} \hat{u}(x_i) \, .$$

$$H_0 = \sum_{rs} \langle r | \hat{z} + \hat{u} | s \rangle \times X_r^\dagger X_s .$$

We will choose our single-particle states such that

$$(\hat{z} + \hat{u}) | p \rangle = \varepsilon_p | p \rangle .$$

(in first quantization,

$$[\hat{z}(x) + \hat{u}(x)] \chi_p(x) = \varepsilon_p \chi_p(x))$$

With these choices

$$H_0 = \sum_r \varepsilon_r X_r^\dagger X_r$$

and every determinant

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

is an eigenstate of H_0.

This can be demonstrated in two ways (see video 32).

Here, we will use an elementary proof based on first quantization.

$$H_0 |\Phi_{q_1 \dots q_N}\rangle$$

$$= \sum_{i=1}^{N} \left[\hat{z}(x_i) + \hat{u}(x_i)\right]$$

$$\times \sqrt{N!}\, A \left(\varphi_{q_1}(x_1) \dots \varphi_{q_N}(x_N)\right)$$

$$= \sqrt{N!}\, A \sum_{i=1}^{N} \left[\hat{z}(x_i) + \hat{u}(x_i)\right]$$

$$\times \varphi_{q_1}(x_1) \dots \varphi_{q_i}(x_i) \dots \varphi_{q_N}(x_N)$$

$$\left[\hat{z}(x_i) + \hat{u}(x_i)\right]\psi_{q_i}(x_i)$$
$$= \varepsilon_{q_i}\psi_{q_i}(x_i)$$

$$H_0 \left|\Phi_{q_1 \dots q_N}\right\rangle = \sqrt{N!}\,\mathcal{A}$$
$$\times \sum_{i=1}^{N} \varepsilon_{q_i} \psi_{q_1}(x_1) \dots \psi_{q_N}(x_N)$$

$$= \left(\sum_{i=1}^{N} \varepsilon_{q_i}\right) \left|\Phi_{q_1 \dots q_N}\right\rangle$$

$$H_0 \left|\Phi_{q_1 \dots q_N}\right\rangle = E^{(0)}_{q_1 \dots q_N} \left|\Phi_{q_1 \dots q_N}\right\rangle$$

$$E^{(0)}_{q_1\cdots q_N} = \sum_{\gamma=1}^{N} \varepsilon_{q_\gamma}$$

In particular, for

0th order IPM state, reference determinant

$$|\Phi_0\rangle = |\Phi_{p_1\cdots p_N}\rangle,$$

$$H_0|\Phi_0\rangle = E^{(0)}_{p_1\cdots p_N}|\Phi_0\rangle$$

$$\equiv E^{(0)}|\Phi_0\rangle,$$

$$E^{(0)} = \sum_{\gamma=1}^{N} \varepsilon_{p_\gamma}$$

What about excited determinants?

$$H_0 |\Phi_{p_\gamma}^{q_\gamma}\rangle = (\varepsilon_{p_1} + \dots + \varepsilon_{p_{\gamma-1}} +$$

$$+ \varepsilon_{q_\gamma} + \varepsilon_{p_{\gamma+1}} + \dots + \varepsilon_{p_N}) |\Phi_{p_\gamma}^{q_\gamma}\rangle$$

$$= [(\varepsilon_{q_\gamma} - \varepsilon_{p_\gamma}) + \varepsilon_{p_1} + \dots \varepsilon_{p_{\gamma-1}} +$$

$$+ \varepsilon_{p_\gamma} + \varepsilon_{p_{\gamma+1}} + \dots + \varepsilon_{p_N}] |\Phi_{p_\gamma}^{q_\gamma}\rangle$$

$$= [(\varepsilon_{q_\gamma} - \varepsilon_{p_\gamma}) + E^{(0)}] |\Phi_{p_\gamma}^{q_\gamma}\rangle$$

$i, j, \ldots \to$ occupied in $|\Phi_0\rangle$ (hole states)

$a, b, \ldots \to$ unoccupied in $|\Phi_0\rangle$ (particle states)

$$H_0 |\Phi_i^a\rangle = \left[(\varepsilon_a - \varepsilon_i) + E^{(0)}\right] |\Phi_i^a\rangle$$

Similarly,

$$H_0 |\Phi_{ij}^{ab}\rangle = \left[(\varepsilon_a - \varepsilon_i + \varepsilon_b - \varepsilon_j)\right.$$

$$+E^{(0)}\Big]\,|\Phi_{ij}^{ab}\rangle,$$

$$H_0|\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}\rangle \quad \checkmark$$

$$=\Big[\sum_{j=1}^{n}(\varepsilon_{a_j}-\varepsilon_{i_j})+E^{(0)}\Big]\times|\Phi_{i_1,\ldots,i_n}^{a_1\ldots a_n}\rangle$$

We define

$$K_0=H_0-\underbrace{\langle\Phi_0|H_0|\Phi_0\rangle}_{E^{(0)}|\Phi_0\rangle}$$

$$(\; K = H_N = H - \langle \Phi_0 | H | \Phi_0 \rangle)$$

$$K_0 = H_0 - E^{(0)}$$

$$K_0 | \Phi_0 \rangle = \varkappa_0 | \Phi_0 \rangle$$

$$K_0 | \Phi_i^a \rangle = \varkappa_i^a | \Phi_i^a \rangle$$

$$\dots$$

$$K_0 | \Phi_{i_1 \dots i_n}^{a_1 \dots a_n} \rangle = \varkappa_{i_1 \dots i_n}^{a_1 \dots a_n} | \Phi_{i_1 \dots i_n}^{a_1 \dots a_n} \rangle$$

$$\varkappa_0 = 0$$

$$\varkappa_i^a = \varepsilon_a - \varepsilon_i$$

$$\dots$$

$$\varkappa_{i_1 \dots i_n}^{a_1 \dots a_n} = \sum_{\gamma=1}^{n} \left(\varepsilon_{a_\gamma} - \varepsilon_{i_\gamma} \right)$$

$$K_0 = H_0 - \langle \Phi_0 | H_0 | \Phi_0 \rangle$$

$$= Z + U - \langle \Phi_0 | Z + U | \Phi_0 \rangle$$

$$= Z_N + U_N = (Z + U)_N$$

$$K_0 = \sum_{r,s} \langle r | \hat{z} + \hat{u} | s \rangle \times N[X_r^\dagger X_s]$$

$$= \sum_r \varepsilon_r N[X_r^\dagger X_r]$$

Example of $\hat{u}$:

$$\hat{u} = \hat{g}$$

$$\hat{z} + \hat{u} = \hat{f}$$

$$\hat{f}|p\rangle = \varepsilon_p |p\rangle.$$

(MBPT $\longrightarrow$ MPPT)

PERTURBATION

$$K = K_0 + W$$

$$W = K - K_0$$

$$K = H_N = H - \langle \Phi_0 | H | \Phi_0 \rangle$$

$$K_0 = H_0 - \langle \Phi_0 | H_0 | \Phi_0 \rangle$$

$$W = H - H_0 - \langle \Phi_0 | H - H_0 | \Phi_0 \rangle$$

$$H = Z + V, \quad H_0 = Z + U$$

$$W = (\cancel{Z} + V) - (\cancel{Z} + U)$$

$$- \langle \Phi_0 | (\cancel{Z} + V) - (\cancel{Z} + U) | \Phi_0 \rangle$$

$$= V - U - \langle \Phi_0 | V - U | \Phi_0 \rangle$$

$$= V_N + G_N - U_N$$

$$W = W_1 + W_2$$

$$W_1 = G_N - U_N \equiv Q_N$$

$$W_2 = V_N$$

$$W_1 = Q_N = \sum_{r,s} \langle r|\hat{q}|s\rangle \times N[X_r^\dagger X_s]$$

$$\hat{q} = \hat{g} - \hat{u}$$

$$\langle r|\hat{q}|s\rangle = \langle r|\hat{g}|s\rangle - \langle r|\hat{u}|s\rangle$$

$$\langle r|\hat{g}|s\rangle = \sum_i \langle ri|\hat{v}|si\rangle_A$$

$$W_2 = V_N = \frac{1}{2}\sum_{rstu} \langle rs|\hat{v}|tu\rangle \times N[X_r^\dagger X_s^\dagger X_u X_t]$$

$$W_1 = Q_N = G_N - U_N$$

$$= Z_N + G_N - (Z_N + U_N)$$

$$= F_N - (Z + U)_N$$

$$F_N = \sum_{r,s} \langle r | \hat{f} | s \rangle N[X_r^\dagger X_s]$$

$$\hat{f} = \hat{z} + \hat{g}$$

$$W_1 = Q_N = \sum_{r,s} \left[\langle r | \hat{f} | s \rangle - \langle r | \hat{z} + \hat{u} | s \rangle \right] N[X_r^\dagger X_s]$$

$$\langle r|\hat{z}+\hat{u}|s\rangle = \varepsilon_r \delta_{rs}$$

$$W_1 = Q_N =$$

$$= \sum_{r,s} \left[\langle r|\hat{f}|s\rangle - \varepsilon_r \delta_{rs} \right] \times N[X_r^\dagger X_s]$$

If $|\Phi_0\rangle$ is a Hartree-Fock determinant,

$$\hat{u} = \hat{g}, \quad \hat{z} + \hat{u} = \hat{f}$$

$$\hat{q} = \hat{g} - \hat{u} = 0,$$

$$W_1 = Q_N = O,$$

$$W = V_N,$$

$$K_0 = Z_N + U_N$$

$$= Z_N + G_N$$

$$= F_N,$$

$$H_N = K = K_0 + W$$

$$= F_N + V_N$$

(MPPT)

MP → Møller-Plesset

(MP2, MP3, MP4, ...)

In general, in MBPT,

$$K_0 = Z_N + U_N \quad \checkmark$$

$$W = W_1 + W_2 , \quad \checkmark$$

$$W_1 = Q_N = G_N - U_N$$

$$\left(= F_N - (Z + U)_N \right)$$

$$W_2 = V_N ,$$

MBPT(2), MBPT(3), MBPT(4), ...

REDUCED RESOLVENT $R^{(0)}$

$$R^{(0)} = \sum_{n \neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{\varepsilon_0 - \varepsilon_n}$$

$$K_0 |\Phi_0\rangle = 0 \quad (\varepsilon_0 = 0)$$

$$K_0 |\Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n}\rangle = \varepsilon_{i_1 \ldots i_n}^{a_1 \ldots a_n} |\Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n}\rangle,$$

$$\varkappa^{a_1\ldots a_n}_{i_1\ldots i_n} = \sum_{j=1}^{n} \left(\varepsilon_{a_j} - \varepsilon_{i_j}\right)$$

$$R^{(2)} = \sum_{n=1}^{N} R^{(2)}_n \qquad \checkmark$$

$$R^{(2)}_n = \sum_{\substack{i_1<\ldots<i_n \\ a_1<\ldots<a_n}} \frac{\left|\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}\right\rangle\left\langle\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}\right|}{\underbrace{-\varkappa^{a_1\ldots a_n}_{i_1\ldots i_n}}_{\sum_{j=1}^{N}\left(\varepsilon_{i_j} - \varepsilon_{a_j}\right)}}$$

$$= \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1 \neq \cdots \neq i_n \\ a_1 \neq \cdots \neq a_n}} \frac{\left| \Phi_{i_1 \cdots i_n}^{a_1 \cdots a_n} \right\rangle \left\langle \Phi_{i_1 \cdots i_n}^{a_1 \cdots a_n} \right|}{-\varepsilon_{i_1 \cdots i_n}^{a_1 \cdots a_n}}$$

We will now allow

EPV terms,

exclusion principle violating

$$R_n^{(0)} = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1, \ldots, i_n \\ a_1, \ldots, a_n}} \frac{\left| \Phi_{i_1 \cdots i_n}^{a_1 \cdots a_n} \right\rangle \left\langle \Phi_{i_1 \cdots i_n}^{a_1 \cdots a_n} \right|}{-\varepsilon_{i_1 \cdots i_n}^{a_1 \cdots a_n}}$$

$$[R^{(0)}]^k = \sum_{n\neq 0} \frac{|\Phi_n\rangle\langle\Phi_n|}{(\mathcal{E}_0-\mathcal{E}_n)^k}$$

$$[R^{(0)}]^k = \sum_{n=1}^{N} [R^{(0)}_n]^k$$

$$[R^{(0)}_n]^k =$$

$$= \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,\ldots,i_n \\ a_1,\ldots,a_n}} \frac{|\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}\rangle\langle\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}|}{\left(-\mathcal{E}^{a_1\ldots a_n}_{i_1\ldots i_n}\right)^k}$$

$$k \geq 1$$

$$\left[R_n^{(0)}\right]^k = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1 \ldots i_n \\ a_1 \ldots a_n}} \frac{E^{a_1 \ldots a_n}_{i_1 \ldots i_n} \overbrace{[\Phi_0 X \Phi_0]} \left(E^{a_1 \ldots a_n}_{i_1 \ldots i_n}\right)^\dagger}{\left(-\epsilon^{a_1 \ldots a_n}_{i_1 \ldots i_n}\right)^k}$$

$$E^{a_1 \ldots a_n}_{i_1 \ldots i_n} = \prod_{g=1}^{n} X^\dagger_{a_g} X_{i_g}$$

$$= \prod_{g=1}^{n} E^{a_g}_{i_g}$$

$$E^a_i = X_a^\dagger X_i$$