Lecture FYS4480/9480, September 20, 2024

FYS4480/9480 lecture September 20

particle-hole formalism

$$|0\rangle \rightarrow |\Phi_0\rangle = \prod_{i=1}^{N} a_i^{\dagger} |0\rangle$$

$$a_p a_q^{\dagger} = \delta_{pq} \qquad pq > F$$

$$a_p^{\dagger} a_q = \delta_{pq} \qquad pq \leq F$$

$$\hat{H} = \hat{F}_N + \hat{V}_N + E_0^{Ref}$$

$$E_0^{Ref} = \langle \Phi_0 | H | \Phi_0 \rangle$$

1p1h : $|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle$

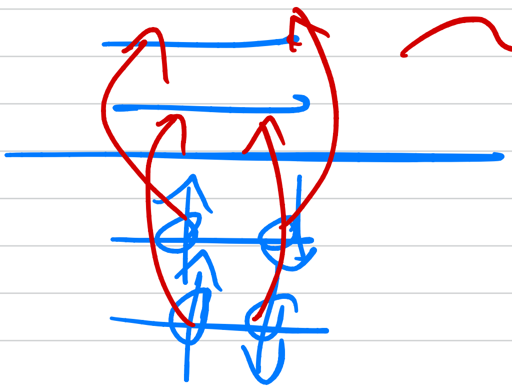
2p2h : $|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle$

$|\Phi_H^P\rangle$ P = n-particle states

H = n-hole states

$n = 0, 1, 2, \ldots N$

Example



~ 4p4h

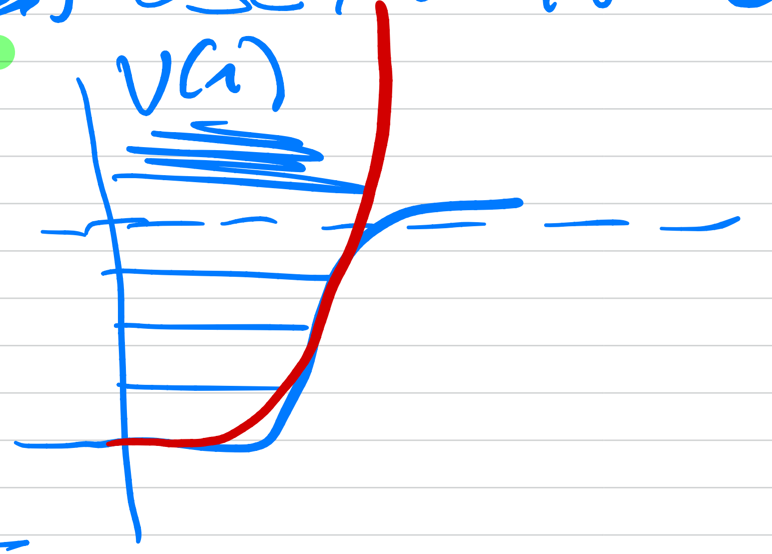
F

0p-0h $|\Phi_0\rangle$

Example: ^{16}O harmonic oscillator

8 protons 8 neutrons

$1p0f$ 20 $\qquad$ $1p0f$ 20



$1s0d$ 12 $\qquad$ $1s0d$ 12

F

$0p$ $\qquad$ $0p$

$n_x=1$ $\quad$ $n_y=1$ $\quad$ $n_z=1$

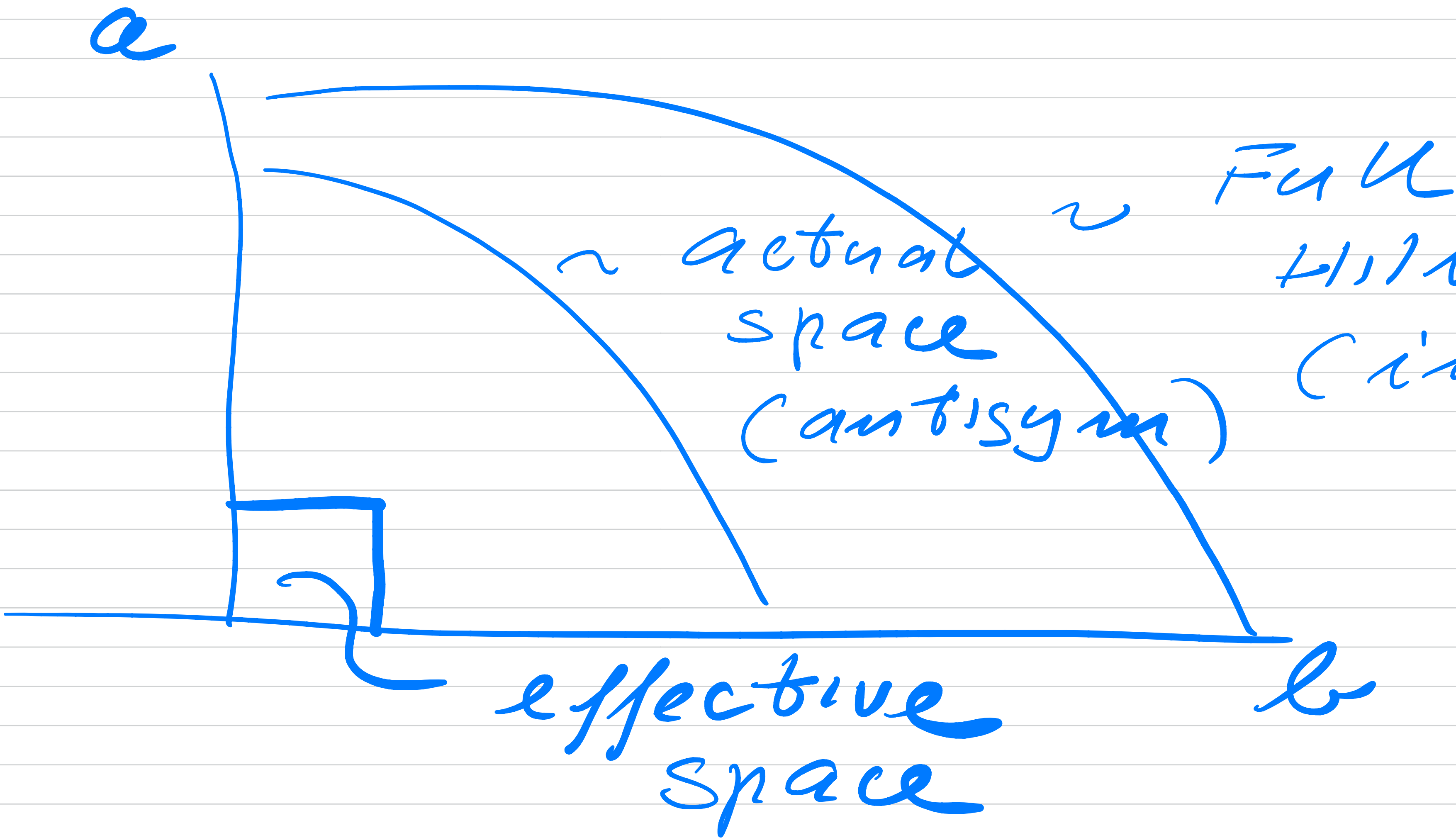
$0s$ $\qquad$ $0s$

protons $\qquad$ neutrons

$n_x=n_y=n_z=0$

proton configs $= \binom{40}{8}$

$$= \frac{40!}{32!\,8!} \sim 10^9$$



$$\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle = ?$$

$$\hat{H} = \hat{F}_N + \hat{V}_N + E_0^{Ref}$$

$$\hat{F}_N = \sum_{pq} \langle p | f | q \rangle \{ a_p^\dagger a_q \}$$

$$\langle p | f | q \rangle = \langle p | h_0 | q \rangle + \sum_i \langle pi | v | qi \rangle_{AS}$$

$$\hat{V}_N = \frac{1}{4} \sum_{pqrs} \langle pq | v | rs \rangle_{AS} \times \{ a_p^\dagger a_q^\dagger a_s a_r \}$$

$$\langle \Phi_0 | F_N | \Phi_i^a \rangle = \langle i | g | a \rangle$$

$$\langle \Phi_0 | V_N | \Phi_i^a \rangle = 0$$

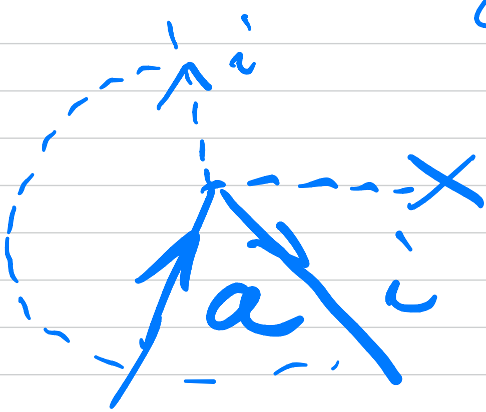
$$\langle \Phi_0 | H | \Phi_i^a \rangle = \boxed{\langle i | g | a \rangle}$$

$$\langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle = \langle ij | v | ab \rangle_{AS}$$

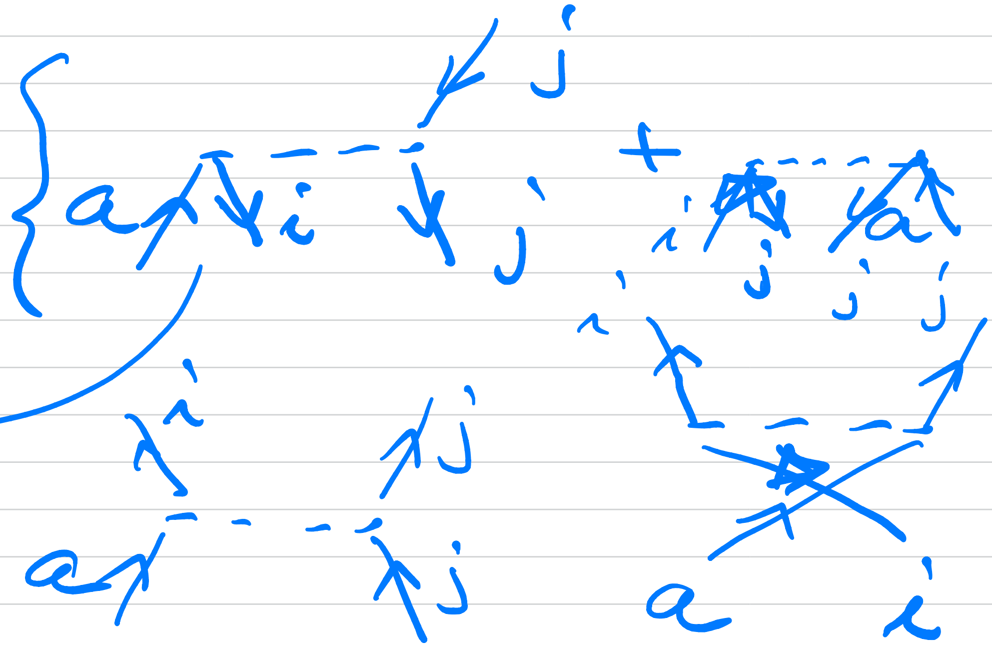
Diagrammatic notation

$a \uparrow \qquad i \downarrow$

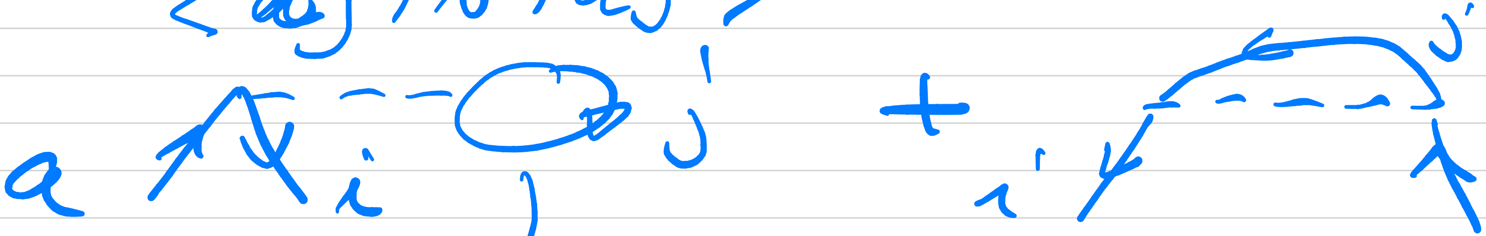
$$\langle i|f|a\rangle = \langle i|h_0|a\rangle + \sum_{j\le F}\langle ij|v|aj\rangle_A$$



$$+ \sum_j \Big\{$$



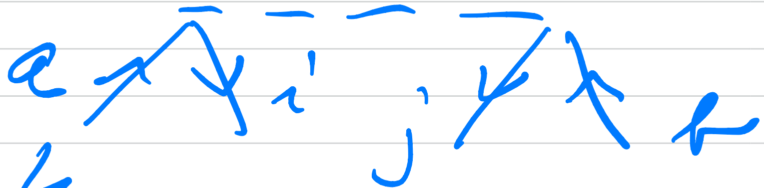
$$\langle aj|v|aj\rangle$$



one closed loop (-1)

one internal (-1)

$$\langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle = \langle ij | v | ab \rangle$$



2p2h
excitation

Exercise :

$$\langle \Phi_i^a | H | \Phi_j^b \rangle \qquad \begin{matrix} i \neq j \\ a \neq b \end{matrix} \text{ or}$$

$$\langle \Phi_0 | a_i^\dagger a_a \underbrace{H}_{E_0^{Ref} + \hat{F}_N + \hat{U}_N} a_b^\dagger a_j | \Phi_0 \rangle$$

$$\hat{F}_N : \{a_p^\dagger a_q\} \qquad \hat{U}_N : \{a_p^\dagger a_q^\dagger a_s a_r\}$$

$$\delta_{ab}\, \delta_{ij}\, E_0^{Ref}$$

$$\hat{F}_N : \quad a_i^\dagger a_a a_p^\dagger a_q a_b^\dagger a_j \quad \sim \langle a|f|b\rangle$$

$$- \langle j|f|i\rangle$$

FCI

Ground state

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$H_0|\Phi_0\rangle = \varepsilon_0|\Phi_0\rangle$$

$$\langle\Phi_i|\Phi_j\rangle = \delta_{ij} \quad \text{(ONS)}$$

$$|\Psi_0\rangle = \sum_{\lambda=0}^{\infty} c_{0\lambda}|\Phi_\lambda\rangle$$

$$c_{0\lambda} = \langle\Psi_0|\Phi_\lambda\rangle$$

$$|\Psi_0\rangle = \sum_{PH} C_H^P \, |\Phi_H^P\rangle$$

$$|\Phi_H^P\rangle = \underbrace{A_H^P}\, |\Phi_0\rangle$$

$$|\Phi_{ij}^{ab}\rangle = \underbrace{a_a^\dagger a_b^\dagger a_j a_i}\, |\Phi_0\rangle$$

$$|\Psi_0\rangle = \underbrace{C_0 |\Phi_0\rangle}_{\text{opgoh}} + \sum_{ai} C_i^a a_a^\dagger a_i |\Phi_0\rangle$$

$$+ \sum_{\substack{ab \\ ij}} C_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle$$

$$+ \ldots + NPNh$$

intermediate normalization

$$\langle \Phi_0 | \Phi_0 \rangle = 1$$

$$\langle \Phi_0 | \Psi_0 \rangle = C_0 = 1$$

$$\sum_{PH} |C_H^P|^2 = 1$$

$$|\Psi_0\rangle = |\Phi_0\rangle + \hat{C}|\Phi_0\rangle$$

$$= (1 + \hat{C})|\Phi_0\rangle$$

$$\hat{C} = \sum_{ai} c_i^a a_a^\dagger a_i + \sum_{\substack{ab \\ ij}} c_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \dots NPNH$$

$$\hat{H}|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$= E_0 \sum_{PH} C_H^P |\Phi_H^P\rangle$$

$\langle\Psi_0| \times$

$$\langle\Psi_0|H|\Psi_0\rangle = \sum_{\substack{PH \\ P'H'}} C_H^{*P} C_{H'}^{P'}$$

$$\times \langle\Phi_H^P|H|\Phi_{H'}^{P'}\rangle = E_0 \sum_{PH} |C_H^P|^2$$

$$\langle\Phi_H^P|\Phi_{H'}^{P'}\rangle = \delta_{PP'}\delta_{HH'}$$

$$\mathcal{L}\left(c^{*P}_{H}, c^{P}_{H}\right) =$$

$$\sum_{\substack{PH \\ P'H'}} c^{*P}_{H} c^{P'}_{H'} \langle \Phi^{P}_{H} | H | \Phi^{P'}_{H'} \rangle$$

$$- \varepsilon_0 \sum_{PH} |c^{P}_{H}|^2$$

$$\uparrow$$

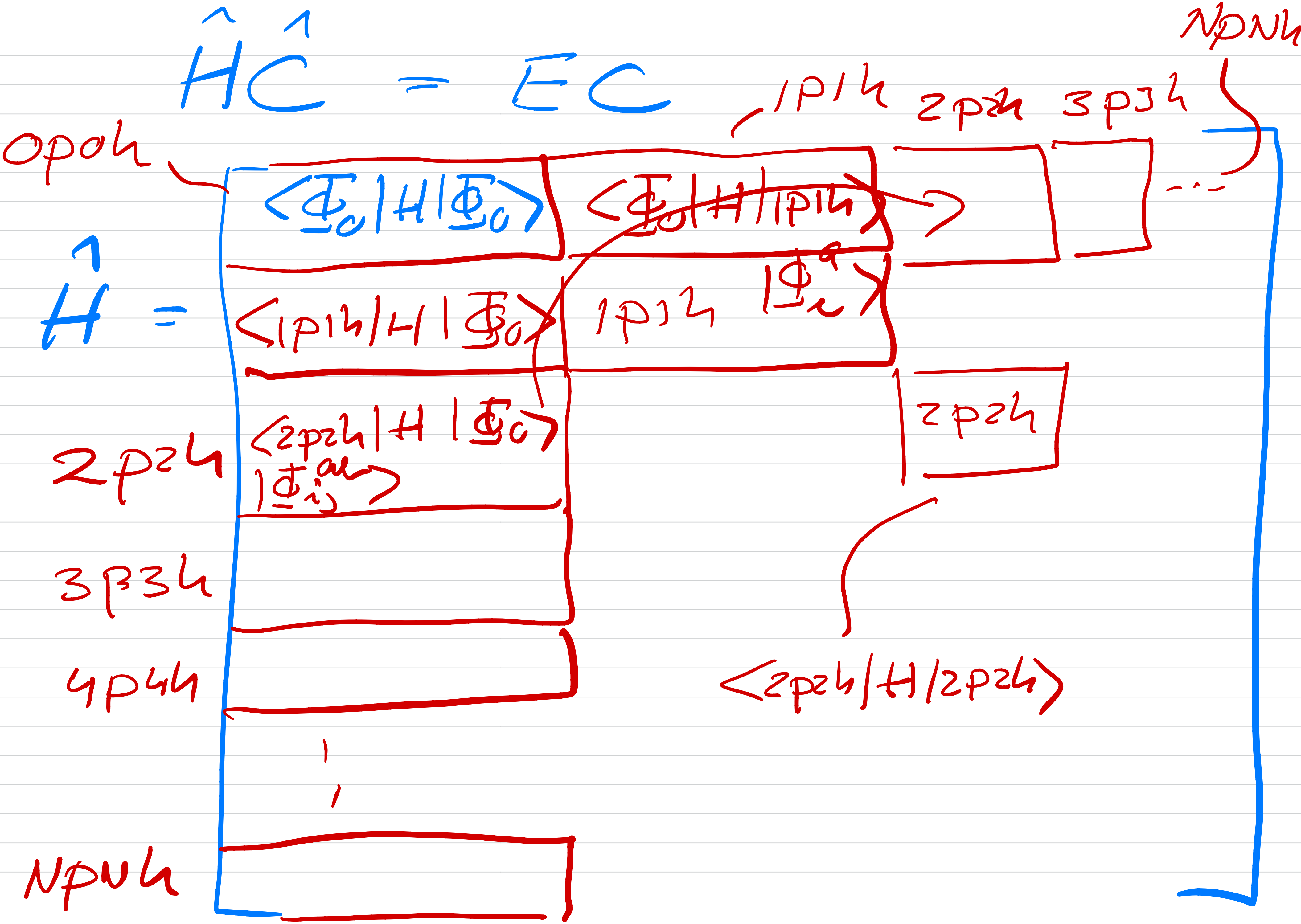
$$c^{*P}_{H} c^{P}_{H}$$

$$\frac{\partial \mathcal{L}}{\partial c^{*P}_{H}} = 0$$

$$\sum_{P'H'} c^{P'}_{H'} \langle \Phi^{P}_{H} | H | \Phi^{P'}_{H'} \rangle = \varepsilon_0 c^{P}_{H}$$

$$\hat{H}\hat{C} = EC$$

$$\hat{H} =$$



$$\langle \Phi_0 | H | \Phi_0 \rangle = E_0^{Ref}$$

$$\langle \Phi_0 | H | \Phi_i^a \rangle = \langle i | f | a \rangle$$

$$\langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle = \langle ij | v | ab \rangle_{AS}$$

H contains at most two-body operator

$$\langle \Phi_0 | H | \underbrace{\Phi_{ijk}^{abc}}_{3p3h} \rangle = 0$$

$$\langle \Phi_0 | H | npnh \rangle = 0 \quad \text{if } n > 2$$

$$\langle 1p1u | H | 2p2u \rangle = 0$$

$$\langle 1p1u | H | npnu \rangle = 0 \text{ if } n \geq 4$$

$$\langle 2p2u | H | 5p5u \rangle = 0$$

$S^T H S = D$

$$
\begin{array}{c|ccccccc}
 & 0p0k & 1p1k & 2p2k & 3p3k & 4p4k & \cdots & NpNk \\
\hline
0p0k & \times & \times & \times & 0 & 0 & \cdots & 0 \\
1p1k & \times & \times & \times & \times & 0 & \cdots & 0 \\
2p2k & \times & \times & \times & \times & \times & 0 \cdots & 0 \\
3p3k & 0 & \times & \times & \times & \times & \times \cdots & 0 \\
4p4k & 0 & 0 & \times & \times & & & \\
\vdots & \vdots & \vdots & 0 & \times & & & \\
\vdots & \vdots & \vdots & \vdots & & & & \\
NpNk & 0 & 0 & \vdots & & & &
\end{array}
$$

Motivation for approximations to FCI

- HF-theory
- Many-body perturbation theory
- Coupled-cluster theory
- Green's function

⋮

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle \Rightarrow$$

$$(H-E_0)\sum_{PH} C_H^P \,|\Phi_H^P\rangle = 0$$

$$\langle \Phi_0 | \times \qquad \langle \Phi_0 | H | \Phi_0 \rangle = E_0^{Ref}$$

$$\langle \Phi_0 | H - E_0 | \Phi_0 \rangle +$$

$$\sum_{ai} C_i^a \langle \Phi_0 | H - E_0 | \Phi_i^a \rangle$$

$$+ \sum_{\substack{ab \\ ij}} C_{ij}^{ab} \langle \Phi_0 | H - E_0 | \Phi_{ij}^{ab} \rangle$$

$$= 0$$

$$\underbrace{E_0 - E_0^{ref}}_{\Delta E} = \sum_{ai} c_i^a \underbrace{\langle \Phi_0 | H | \Phi_i^a \rangle}_{\langle i | g | a \rangle}$$

correlation energy

$$+ \sum_{\substack{ab \\ ij}} c_{ij}^{ab} \underbrace{\langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle}_{\langle ij | v | ab \rangle}$$

$$= \sum_{ai} c_i^a \langle i | g | a \rangle + \sum_{\substack{ab \\ ij}} c_{ij}^{ab} \langle ij | v | ab \rangle$$

MBPT(2)

HF $= 0$

$$c_i^a = \frac{\langle a | g | i \rangle}{\varepsilon_i - \varepsilon_a}$$

$$\frac{\langle ab | v | ij \rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$