FYS4480/9480, lecture
October 9, 2025

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$$|\Phi_0^{HF}\rangle = |c\rangle$$

$$|c'\rangle = |c\rangle + |\delta c\rangle$$

$$|c'\rangle = \exp\left\{\sum_{ai} \delta c_i^a a_a^\dagger a_i\right\}|c\rangle$$

$$E_0^{HF} = \langle c|\mathcal{H}|c\rangle$$

$$\frac{\langle c'|\mathcal{H}|c'\rangle}{\langle c'|c'\rangle} \geq \langle c|\mathcal{H}|c\rangle$$

$$\frac{\langle c' | \mathcal{H} | c' \rangle}{\langle c' | c' \rangle} \simeq E_0^{HF} + \frac{\Delta E}{\underbrace{1 + \sum_{ai} |\delta c_i^a|^2}}$$

$$\Delta E \geq 0$$

$$\langle c' | \mathcal{H} | c' \rangle = E_0^{HF} \Big(\qquad \Big)$$

$$+ \sum_{ai} |\delta c_i^a|^2 (\varepsilon_a^{HF} - \varepsilon_i^{HF}) \qquad (ii)$$

$$+ \sum_{\substack{ab \\ ij}} \delta c_i^{a*} \delta c_j^b \langle aj || ib \rangle_{AS}$$

1PIh

$$+\frac{1}{2}\sum_{\substack{ai\\bj}} \delta c_i^{a}\,\delta c_j^{b}\,\langle ij|v|ab\rangle_{AS} \quad (ii)$$

$$+\frac{1}{2}\sum_{\substack{ai\\bj}} \delta c_i^{*a}\,\delta c_j^{*b}\,\langle ab|v|ij\rangle_{AS} \quad (iii)$$

$$\langle 0p0h|H|2p2h\rangle$$

<u>First one</u>

(i)

$$\sum_{\substack{ab\\ij}} \delta^* C_i^a \, \delta C_j^b \Big\{ \big[\varepsilon_a^{HF} \delta_{ab} \delta_{ij} - \varepsilon_i^{HF} \delta_{ab} \delta_{ij} \big] + \langle aj || ib \rangle_{AS} \Big\}.$$

$I = \{ai\}$ 1p1h excitation

$J = \{bj\}$ — " —

$$\underline{\langle aj || ib \rangle}_{AS} = A_{ai,bj} = A_{IJ}$$

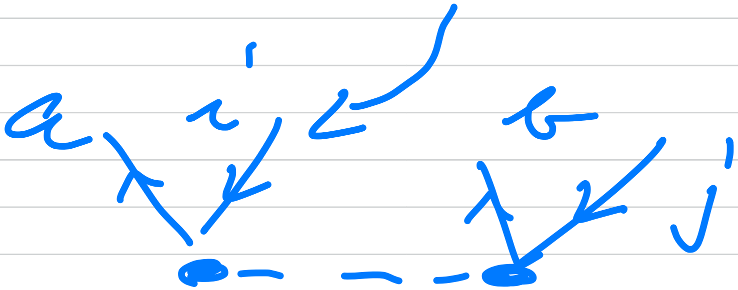
$$\delta^* C_i^a = \delta^* C_I$$

$$\delta c_j^b = \delta c_J$$

$$\Delta E_{IJ} = (\epsilon_a^{HF} - \epsilon_i^{HF})\,\delta_{ab}\,\delta_{ij}$$

(ii) $\langle ab|v|ij\rangle_{AS} = B_{IJ}$

$$= \langle ab|v|ij\rangle - \langle ba|v|ij\rangle$$



2p2h exca-tations

(iii) $\langle ij|v|ab\rangle_{AS} = B^*_{IJ}$

$$\Delta E = \sum_{IJ} \delta c_I^* \, \delta c_J \left[\Delta \varepsilon_{IJ} \, \delta_{IJ} + A_{IJ} \right]$$

$$\left(x^T A x = \sum_{i,j} x_i \, a_{ij} \, x_j \right)$$

$$+ \sum_{IJ} \delta c_I \, \delta c_J \, B_{IJ}^*$$

$$+ \sum_{IJ} \delta c_I^* \, \delta c_J^* \, B_{IJ}$$

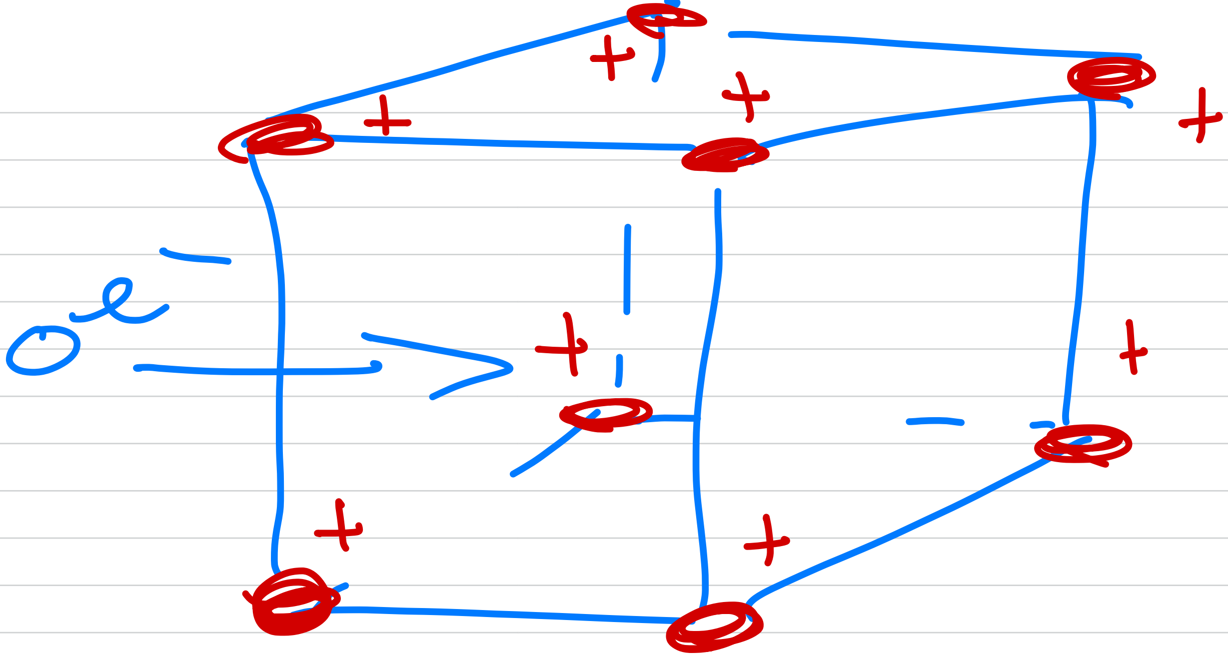
$$\Delta E = \frac{1}{2} \langle X | M | x \rangle \, ; \; X = \begin{bmatrix} \delta c \\ \delta c^* \end{bmatrix}$$

$$M = \begin{bmatrix} \Delta\varepsilon + A & B \\ B^* & \Delta\varepsilon + A^* \end{bmatrix}$$

$\Delta\varepsilon \geq 0$ then M has to be semi-positive definite (eigenvalues $\lambda_i \geq 0$)

A necessary (but not sufficient) condition is that

$$\varepsilon_a^{HF} - \varepsilon_i^{HF} + \langle ai \| ia \rangle_{AS} \geq 0$$



e^-

Electron gas in 3D.

(i) $$\varepsilon_p^{HF} = \langle p | \hat{h}_0 | p \rangle + \sum_{j \le F} \langle pj | v | pj \rangle_{AS}$$

(ii) $$\langle \Phi_0^{HF} | H | \Phi_0^{HF} \rangle = E_0^{HF}$$

$\hat{h}_0 = \hat{t}$ (kinetic energy only)

$$\hat{t} = -\frac{\hbar^2 \nabla^2}{2m}$$

For a particle in box (3D) with infinite walls

$$\vec{k} = \frac{2\pi}{L}\left(n_1 \vec{e}_1 + n_2 \vec{e}_2 + n_3 \vec{e}_3\right)$$

$$n_i = 0, \pm 1, \pm 2, \ldots$$

$$\varphi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\vec{r}}$$

$$\hat{t}\,\varphi_{\vec{k}}(\vec{r}) = \frac{\hbar^2 k^2}{2m}\varphi_{\vec{k}}(\vec{r})$$

$$p^2 = \hbar^2 k^2 \rightarrow$$

$$\langle p | \hat{t} | p \rangle =$$

$$= \frac{1}{\Omega} \int_\Omega d\vec{r}\, \frac{p^2}{2m} |\varphi_p(\vec{r})|^2$$

$$= \frac{p^2}{2m} \frac{1}{\Omega} \int_\Omega d\vec{r}\, e^{i\vec{p}\vec{r}} e^{-i\vec{p}\vec{r}}$$

$$\int d\vec{r}\, \frac{e^{i\vec{p}\vec{r}}}{\sqrt{\Omega}}\, \hat{t}\, \frac{e^{-i\vec{p}\vec{r}}}{\sqrt{\Omega}}$$

$$= \frac{p^2}{2m} \qquad \int_\Omega d\vec{r} = \Omega$$

$p^2 \propto n_1^2 + n_2^2 + n_3^2$, give rise to "magic numbers"

$n_1^2+n_2^2+n_3^2$	n_1	n_2	n_3		$N_{\uparrow\downarrow}$
0	0	0	0		2
1	1	0	0	12	
	-1	0	0		
	0	1	0		
	0	-1	0		12+2
	0	0	1		14
	0	0	-1		
2	-1	-1	0	24	38
	+11 more				
3	-1	-1	-1 ...	16	54

HF-potential

$$\langle p | u^{HF} | p \rangle =$$

$$\sum_{j \leq F} \langle pj | v | pj \rangle - \sum_{j \leq F} \langle pj | v | jp \rangle$$

specific integral $\begin{bmatrix}1 & 0\end{bmatrix} \begin{bmatrix}1 \\ 0\end{bmatrix}$

$$\sum_{j \leq k_F} \sum_{\sigma_j = \pm 1/2} \langle p\sigma_p j\sigma_j' | v | p\sigma_p j\sigma_j \rangle$$

$(1\,0)$ $\begin{bmatrix}1 \\ 0\end{bmatrix}$

independent of spin

σ_p is fixed

$\sigma_j' = 1/2$ $\begin{pmatrix}1 \\ 0\end{pmatrix}$ or $-\frac{1}{2}$ $\begin{pmatrix}0 \\ 1\end{pmatrix}$

$$= 2 \sum_{j \le k_F} \langle pj \, | v | \, pj \rangle$$

Exchange

$$- \sum_{j \le k_F} \sum_{\sigma_j = \pm 1/2} \langle p\sigma_p \, j\sigma_j \, | v | \, j\sigma_j \, p\sigma_p \rangle$$

$$\sigma_p = +1/2 \qquad \xi_{\sigma_p} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\begin{array}{c} \sigma_p \\ \begin{bmatrix} 1 & 0 \end{bmatrix} \end{array} \quad \begin{array}{c} \sigma_j \\ \begin{bmatrix} 1 & 0 \end{bmatrix} \end{array} \quad \begin{array}{c} \sigma_j \\ \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{array} \quad \begin{array}{c} \sigma_p \\ \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{array}$$

1 2 1 2

$$\begin{array}{cccc} \sigma_p & \sigma_j = -1/2 & \sigma_j = -1/2 & \sigma_p \\ \begin{bmatrix} 1 & 0 \end{bmatrix} & \begin{bmatrix} 0 & 1 \end{bmatrix} & \begin{bmatrix} 0 \\ 1 \end{bmatrix} & \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ 1 & 2 & 1 & 2 \end{array}$$

$$= 0$$

$\Rightarrow$ For the exchange term

$$- \sum_{j \le k_F} \langle pj | v | jp \rangle$$

Exchange term

$$\frac{1}{\sqrt{\Omega}} e^{i\vec{k}\vec{r}}$$

$$-\sum_{j\le k_F} \langle pj|v|jp\rangle$$

$$= -\sum_{j\le k_F} \frac{e^2}{\Omega^2} \int d\vec{r} \int d\vec{r}\,'$$

$$\times \frac{e^{i(\vec{j}-\vec{p})\vec{r}}\, e^{i(\vec{p}-\vec{j})\vec{r}\,'}}{|\vec{r}-\vec{r}\,'|}$$

Direct term $\underbrace{\qquad}_{}$ $\sum_{j \le k_F} 1 =$

$$\frac{2}{\Omega} \sum_{j \le k_F} \int d\vec{r}\,' \frac{e^2}{|\vec{r} - \vec{r}\,'|}$$

$$= \frac{Ne^2}{\Omega} \int d\vec{r}\,' \frac{e^2}{|\vec{r} - \vec{r}\,'|}$$

This term cancels a term from the Background ions

$$\varepsilon_p^{HF} = \frac{\hbar^2 p^2}{2m} - \text{Exchange term}$$

$p \Rightarrow k \qquad q \Rightarrow k'$

$$-\frac{e^2}{\Omega^2} \sum_{k' \le k_F} \int d\vec{r}\, e^{i(\vec{k}-\vec{k}')\vec{r}}$$

$$\times \int d\vec{r}\,' \frac{e^{i(\vec{k}-\vec{k}')\vec{r}\,'}}{|\vec{r}-\vec{r}\,'|}$$

How do we evaluate the exchange term?

(i) convergence $e^{-\mu|\vec{r}-\vec{r}\,'|}$
evaluate integral, $\lim_{\mu \to 0} I$

(iii) $\frac{1}{\Omega}\sum_{\vec{k}} \longrightarrow \frac{1}{(2\pi)^3}\int d\vec{k}$

$$\frac{e^2}{\Omega(2\pi)^3}\int d\vec{r}\int\frac{d\vec{r}\,'}{|\vec{r}-\vec{r}\,'|}\int d\vec{k}\,'$$

$$\times\, e^{i(\vec{k}\,'-\vec{k})(\vec{r}-\vec{r}\,')}\, e^{-\mu(|\vec{r}-\vec{r}\,'|)}$$