FYS4480 September 1

Repeat from week 34

$$\varphi_\alpha(x) = \langle x|\alpha\rangle$$

$$\int dx = \sum_{m_s} \int d^d r$$

$$= \sum_{m_s} \int d\vec{r}$$

one-body operator

$$\hat{h}_0(x) = \hat{t}(x) + \hat{v}_{ext}(x)$$

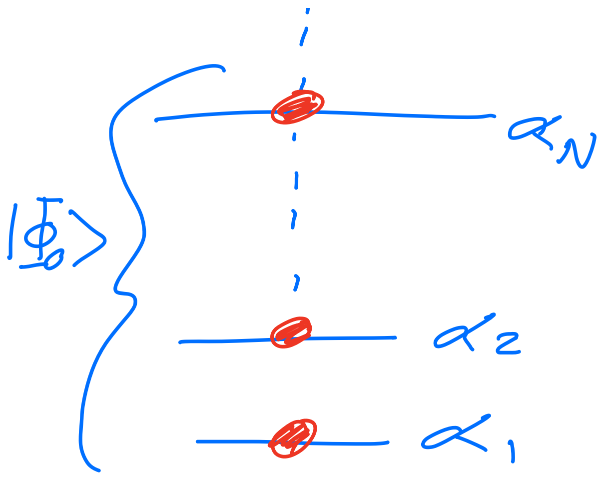
kinetic energy

$$\hat{h}_0(x)\varphi_\alpha(x) = \varepsilon_\alpha \varphi_\alpha(x)$$

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}_0(x_i)$$

$$\hat{H}_I = \sum_{i<j}^{N} v(x_i, x_j)$$



sp states

$\varepsilon_1 < \varepsilon_2 < \varepsilon_3 \ldots$

ansatz for $|\Phi_0\rangle$

$$|\Phi_0\rangle \longrightarrow \Phi_0(x_1\, x_2 \ldots x_N ; \alpha_1, \ldots \alpha_N)$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_1}(x_1) & \cdots & \varphi_{\alpha_1}(x_N) \\ \varphi_{\alpha_2}(x_1) & & \vdots \\ \vdots & & \vdots \\ \varphi_{\alpha_N}(x_1) & & \varphi_{\alpha_N}(x_N) \end{vmatrix}$$

$$\hat{H}_0 |\Phi_0\rangle = E_0 |\Phi_0\rangle$$

$$E_0 = \sum_{\alpha_i=1}^{N} \varepsilon_{\alpha_i}$$

$[H_0, H_1] \neq 0 \qquad [t, V_{ext}] \neq 0$

$$\Phi_0(\ldots) = \frac{1}{\sqrt{N!}} \sum_P (-)^P P\, \Phi_H$$

$$\Phi_H = \varphi_{\alpha_1}(x_1)\,\varphi_{\alpha_2}(x_2) \cdots \varphi_{\alpha_N}(x_N)$$

Hartree function.

$\underline{N=2}$

$$\frac{1}{\sqrt{2!}}\left(\varphi_{\alpha_1}(x_1)\varphi_{\alpha_2}(x_2) - \varphi_{\alpha_1}(x_2)\varphi_{\alpha_2}(x_1)\right)$$

Introduce

$$\hat{A} = \frac{1}{A!} \sum_P (-)^P \hat{P}$$

$A=2$

$$\hat{A} = (1 - P_{12})\frac{1}{2} \qquad \Big|\ \hat{A}\, \underbrace{\varphi_{\alpha_1}(x_1)\varphi_{\alpha_2}(x_2)}_{x_1 \leftrightarrow x_2}$$

$$\hat{A}^2 = (1 - P_{12})\frac{1}{2}\,\frac{1}{2}(1 - P_{12})$$

$$= \frac{1}{4}(1 - 2P_{12} + P_{12}^2)$$

$$= \hat{A} \qquad \hat{A} = \hat{A}^{+}$$

$$[H_0, \hat{A}] = 0$$

one-body

$$[H_I, \hat{A}] = 0$$

$$v(x_i, x_j) = v(|x_i - x_j|) = v(x_{ij})$$

$$= v(|x_j - x_i|)$$

$$\langle \Phi_0 | \hat{H} | \Phi_0 \rangle =$$

$$\langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle + \langle \Phi_0 | H_I | \Phi_0 \rangle$$

$$\langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle = ?$$

$$d\tau = dx_1 \, dx_2 \dots dx_N$$

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \int d\tau \, \Phi_0^* \hat{H}_0 \Phi_0$$

$$= N! \int \Phi_H^* \underbrace{\hat{A} H_0}_{\hat{H}_0 \hat{A}} \hat{A} \Phi_H \, d\tau$$

$$\left(\begin{aligned} \hat{A} &= \frac{1}{N!} \sum_P (-1)^P \hat{P} \\ \Phi_0 &= \frac{1}{\sqrt{N!}} \left| \cdots \right| \end{aligned} \right)$$

$$= \cancel{N}! \int d\tau \, \Phi_H^* \hat{H}_0 \cancel{\hat{A}} \Phi_H$$

$$= \int d\tau \, \Phi_H^* \hat{H}_0 \sum_P (-1)^P \hat{P} \Phi_H$$

$$= \int dx_1 dx_2 \cdots dx_N \, \varphi_{\alpha_1}^*(x_1) \varphi_{\alpha_2}^*(x_2) \cdots \varphi_{\alpha_N}^*(x_N) \left(h_0(x_1) + h_0(x_2) + \cdots \right)$$

$$\times \left(\varphi_{\alpha_1}(x_1) \varphi_{\alpha_2}(x_2) \cdots \varphi_{\alpha_N}(x_N) \right)$$

$$(|\alpha_1 x_1\rangle\, |\alpha_2 x_2\rangle \cdots |\alpha_N x_N\rangle$$

$$+ \text{ all permutations })$$

$$\int dx_i'\, \varphi^*_{\alpha_i'}(x_i')\, \varphi_{\alpha_1}(x_1') = \underline{1}$$

$$\hat{h}_0 \varphi_{\alpha_i'} = \varepsilon_{\alpha_1'} \varphi_{\alpha_1'}$$

$$= \sum_{\alpha_i'=1}^{N} \varepsilon_{\alpha_i'}$$

all permutations

$$\begin{matrix} P_{12} & P_{13} & \cdots & P_{1N} \\ & P_{23} & \cdots & P_{2N} \\ & & P_{34} \cdots & P_{3N} \\ & & & \ddots \end{matrix}$$

$$= 0$$

$$\int dx_1 dx_2\, \varphi^*_{\alpha_1}(x_1)\, \varphi^*_{\alpha_2}(x_2)\, \big(h_0(x_1) + h_0(x_2)\big)$$

$$\times\, \varphi_{\alpha_1}(x_2)\, \varphi_{\alpha_2}(x_1)\Big)$$

$$\times \underbrace{\int dx_3\, \varphi^*_{\alpha_3} \varphi_{\alpha_3}}_{=\underline{1}} \cdots \underbrace{\int dx_N}_{=\underline{1}}$$

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \sum_{\alpha_i'=1}^{N} \varepsilon_{\alpha_i'}$$

$$= \sum_{\alpha_i=1}^{N} \langle \alpha_i | \hat{h}_0 | \alpha_i \rangle$$

$$\int dx\, \varphi^*_{\alpha_i}(x)\, \hat{h}_0(x)\, \varphi_{\alpha_i}(x)$$

$\langle \Phi_c | \hat{O} | \Phi_c \rangle$ with

$$\langle \alpha_i | \hat{O} | \alpha_j \rangle = 0$$

$$\langle \Phi_c | H_1 | \Phi_c \rangle =$$

$$\int \Phi_0^* H_I \Phi_0 \, d\tau$$

$$\sum_{i<j} \int d\tau\, \Phi_H^*\, v(x_i, x_j) \sum_P (-)^P \hat{P}\, \Phi_H$$

$$v(|x_i - x_j|)$$

$$\sum_P (-)^P \hat{P} = \left(1 - P_{12} - P_{13} \cdots \right)$$

$$\int dx_1\, dx_2 \cdots dx_N\, \varphi^*_{\alpha_1}(x_1)\, \varphi^*_{\alpha_2}(x_2) \cdots$$

$$v(x_{12})\left(\underline{1} - P_{12} - P_{13} - -\right)$$
$$\times\, \varphi_{\alpha_1'}(x_1)\varphi_{\alpha_2}(x_2)\varphi_{\alpha_3}(x_3)\ldots$$

$$\int dx_1 dx_2\, \varphi^*_{\alpha_1}(x_1)\varphi^*_{\alpha_2}(x_2)\, v(x_{12})$$
$$\times\, \varphi_{\alpha_1}(x_1)\varphi_{\alpha_2}(x_2)\int dx_3\, \varphi^*_{\alpha_3}(x_3)\,\varphi_{\alpha_3}(x_3) = 1$$
$$\ldots \int dx_N - = 1$$

$$\underbrace{\langle \alpha_1\alpha_2 | v | \alpha_1\alpha_2\rangle}_{}$$ Direct term

Exchange

$(1\ 0)\begin{pmatrix}1\\0\end{pmatrix}$

$$-\int dx_1 dx_2\, \varphi^{*\uparrow}_{\alpha_1}(x_1)\varphi^{*\downarrow}_{\alpha_2}(x_2)\, v(x_{12})$$
$$\sum_{m_s}\int d\vec{r}_2 \quad \varphi^{\uparrow}_{\alpha_1}(\underline{x_2})\,\varphi^{\downarrow}_{\alpha_2}(x_1)\int dx_3 \ldots \int dx_N$$

$$\langle \alpha_1\alpha_2 | v | \underline{\alpha_2}\alpha_1\rangle$$

$$-\int dx_1 dx_2 dx_3\, \varphi^*_{\alpha_1}(x_1)\varphi^*_{\alpha_2}(x_2)\varphi^*_{\alpha_3}(x_3)$$
$$\times\, v(x_{12})\,\varphi_{\alpha_1}(x_3)\varphi_{\alpha_2}(x_2)\varphi_{\alpha_3}(x_1)$$
$$\int dx_4 - - -$$

$$\langle \Phi_0 | H_1 | \Phi_0\rangle$$

$$= \sum_{i<j}^{N} \int \Phi_H^* v(x_{ij})(1-P_{ij}) \times \Phi_H \, d\lambda$$

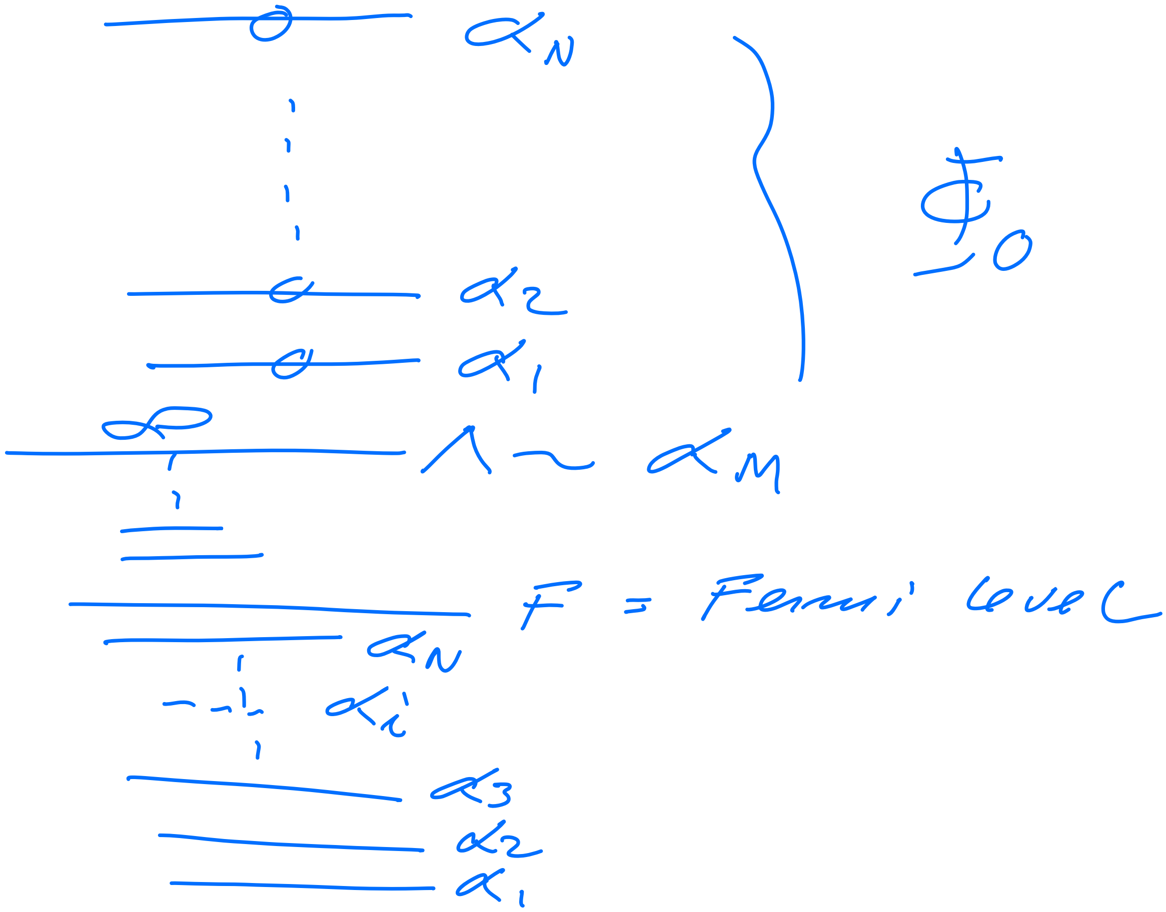
$$= \sum_{\alpha_i < \alpha_j}^{N} \Big(\langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle - \langle \alpha_i \alpha_j | v | \alpha_j \alpha_i \rangle \Big)$$

$$= \frac{1}{2} \sum_{\alpha_i \alpha_j}^{N} \Big(\langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle - \langle \alpha_i \alpha_j | v | \alpha_j \alpha_i \rangle \Big)$$

$$\langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle_{AS} = \langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle - \langle \alpha_i \alpha_j | v | \alpha_j \alpha_i \rangle$$

$$\langle \Phi_0 | \hat{H} | \Phi_0 \rangle$$

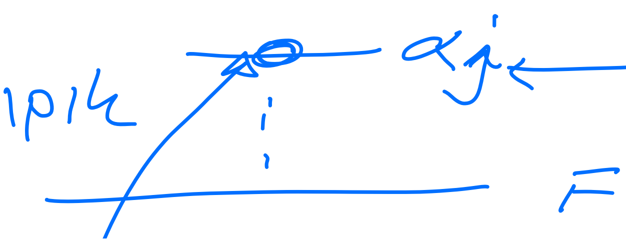
$$\hat{H} \to \hat{O} \qquad \Phi_0 \to \Phi$$

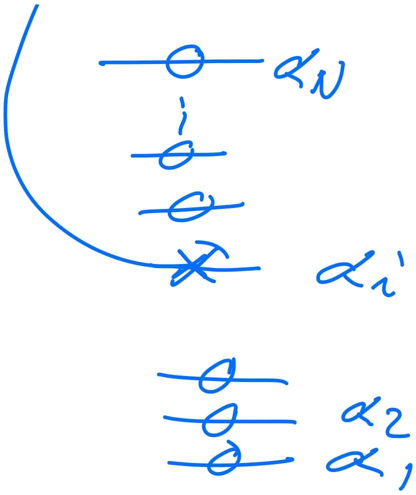


$$\varepsilon_{\alpha_1} < \varepsilon_{\alpha_2} < \varepsilon_{\alpha_3} \cdots < \varepsilon_{\alpha_N} \cdots < \varepsilon_{\alpha_M}$$

$$\Phi_{\alpha_i}^{\alpha_j} \qquad \Phi_0 \propto \varphi_{\alpha_1}\varphi_{\alpha_2}\cdots\varphi_{\alpha_N}$$

$$\Rightarrow \propto \varphi_{\alpha_1}\varphi_{\alpha_2}\cdots\varphi_{\alpha_{i-1}}\varphi_{\alpha_{i+1}}\cdots\varphi_{\alpha_j}$$





$N-1$

True ground state

$$|\Psi_0\rangle = \sum_{i=0}^{\infty} c_{0i} \underbrace{|\Phi_i\rangle}_{\text{computational many-body basis}}$$

$$\langle \Phi_i | \Phi_j \rangle = \delta_{ij}$$

$$\langle \Phi | H | \Phi_{\alpha_i}^{\alpha_j} \rangle$$

$N = 4$

$\underline{H_0} \wedge \underline{H_1}$ $(\hat{O}_1 \text{ or } \hat{O}_2)$

$$\int dx_1\, dx_2\, dx_3\, dx_4\, \varphi^*_{\alpha_1}(x_1)\, \varphi^*_{\alpha_2}(x_2)$$

$$\times \varphi^*_{\alpha_3}(x_3)\, \varphi^*_{\alpha_4}(x_4) \Big(\hat{O}_1(x_1) + \hat{O}_1(x_2)$$

$$+ \hat{O}_1(x_3) + \hat{O}_1(x_4) \Big)$$

$$\times \Big(\varphi_{\alpha_1'}(x_1)\, \varphi_{\alpha_2}(x_2)\, \varphi_{\alpha_3'}(x_3)\, \varphi_{\alpha_4}(x_4)$$

$$+ P_{12} + P_{13} + P_{14} + \dots \Big)$$

$$\alpha_3' \neq \alpha_3$$

$$= \int dx_3\, \varphi^*_{\alpha_3}(x_3)\, \hat{O}_1(x_3)\, \varphi_{\alpha_3'}(x_3)$$

$$= \langle \alpha_3 | \hat{O}_1 | \alpha_3' \rangle$$

$$\hat{O}_1 |\alpha_3\rangle = o_{\alpha_3} |\alpha_3\rangle$$

$$\hat{O} \Rightarrow \hat{O}_2(x_i, x_j)$$