Lecture August 31, 2023, Fys4480/9480

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

$$\alpha = 0, 1, 2, \ldots \infty$$

$$\varepsilon_\alpha \overset{HO}{=} \hbar\omega\,(n_{x\alpha} + n_{y\alpha} + 1) \quad \text{2dim HO}$$

$\alpha - 1$ $\qquad \varphi_{\alpha-1}(\vec{x})$

Fermi level

$\alpha = 3$

$\alpha = 2$ $\qquad \varphi_2(\vec{x})$

$\alpha = 1$ $\qquad \varphi_1(\vec{x})$

$\alpha = 0$ $\qquad \varphi_\alpha(\vec{x}) = \varphi_0(\vec{x})$

$n_{x0}\ n_{y0}$

assume lowest-lying state

$$\Phi_0(\vec{x}_1, \vec{x}_2, \ldots \vec{x}_N; \alpha_0, \alpha_1, \ldots, \alpha_{N-1})$$

$$\propto \boxed{\varphi_{\alpha_0}(\vec{x}_1)\, \varphi_{\alpha_1}(\vec{x}_2) \cdots \varphi_{\alpha_{N-1}}(\vec{x}_N)}$$

$$= \Phi_H(\vec{x}_1, \vec{x}_2, \ldots \alpha_0 \ldots)$$

Hartree product
defined by our ordering
does not obey symmetry requirements

$$\Phi_0(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N ; \alpha_0 \ldots \alpha_{N-1})$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_0}(\vec{x}_1) & \varphi_{\alpha_0}(\vec{x}_2) & \cdots & \varphi_{\alpha_0}(\vec{x}_N) \\ \varphi_{\alpha_1}(\vec{x}_1) & - & - & \vdots \\ \vdots & - & - & \vdots \\ \varphi_{\alpha_{N-1}}(\vec{x}_1) & - & \cdot & \cdot \end{vmatrix}$$

$$= \underbrace{\frac{1}{\sqrt{N!}} \sum_{P=0}^{P!} (-)^P \hat{P}}_{\sqrt{N!}\,\hat{A}} \varphi_{\alpha_0}(\vec{x}_1)\, \varphi_{\alpha_1}(\vec{x}_2) \cdots \varphi_{\alpha_{N-1}}(\vec{x}_N)$$

Define Antisymmetrization operator

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

$N = 2$

$$\hat{A} = \frac{1}{2}\left(1 - \hat{P}_{12}\right)$$

$$\hat{A}^2 = \frac{1}{4}\left(1 - \hat{P}_{12}\right)\left(1 - \hat{P}_{12}\right)$$

$$= \frac{1}{4}\left(1 - 2\hat{P}_{12} + \underbrace{\hat{P}_{12}^2}\right)$$

$$= \frac{1}{2}\left(1 - \hat{P}_{12}\right) \; {}^{2} \; = \hat{A}$$

$$[\hat{H}_0, \hat{A}] = [H_I, \hat{A}] = 0$$

$$\Phi_0(\vec{x}_1 \vec{x}_2 \ldots \vec{x}_N; \alpha_0 \alpha_1 \ldots \alpha_{N-1})$$

$$= \sqrt{N!}\, \hat{A}\, \underbrace{\Phi_H(\vec{x}_1 \vec{x}_2 \ldots \vec{x}_N; \alpha_0 \ldots \alpha_{N-1})}_{\varphi_{\alpha_0}(\vec{x}_1)\, \varphi_{\alpha_1}(\vec{x}_2) \ldots \varphi_{\alpha_{N-1}}(\vec{x}_N)}$$

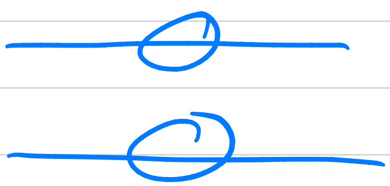
$$\langle \Phi_0 | \hat{H}_0 + \hat{H}_1 | \Phi_0 \rangle$$

last week we did $N = 2$

$$\langle \Phi_0(N=2) | \hat{H}_0 | \Phi_0(N=2) \rangle$$

$$= \varepsilon_{\alpha_0} + \varepsilon_{\alpha_1}$$

$$\Phi_H = \varphi_{\alpha_0}(\vec{x}_1)\,\varphi_{\alpha_1}(\vec{x}_2)$$

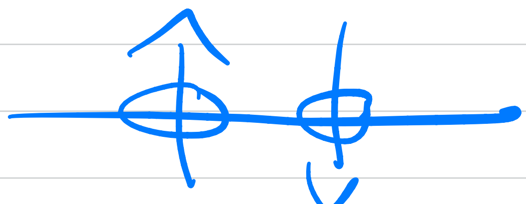


α_1

α_0

with spin
(S=1/2)

$$h_0(x)\,\varphi_{\alpha_i} = \varepsilon_{\alpha_i}\,\varphi_{\alpha_i}$$



α_0 α_1

$$\langle \Phi_0 | H_I | \Phi_0 \rangle$$

$$= \iint dx_1 dx_2 \, \varphi^*_{\alpha_0} \varphi^*_{\alpha_1} \hat{v}(x_1, x_2)$$

$$\times \varphi_{\alpha_0} \varphi_{\alpha_1}$$

$$\underbrace{\langle \alpha_0 \alpha_1 | \hat{v} | \alpha_0 \alpha_1 \rangle}_{\text{Direct term}}$$

$$- \iint dx_1 dx_2 \, \varphi^*_{\alpha_0}(x_2) \varphi^*_{\alpha_1}(x_1) \, v(x_1, x_2)$$

$$\times \varphi_{\alpha_0}(x_1) \varphi_{\alpha_1}(x_2)$$

Exchange $\langle \alpha_1 \alpha_0 | v | \alpha_0 \alpha_1 \rangle$

$$\langle \alpha_0 \alpha_1 | v | \alpha_0 \alpha_1 \rangle = \langle \alpha_1 \alpha_0 | v | \alpha_1 \alpha_0 \rangle$$

$$\langle \alpha_0 \alpha_1 | v | \alpha_1 \alpha_0 \rangle = \langle \alpha_1 \alpha_0 | v | \alpha_0 \alpha_1 \rangle$$

$$\langle \alpha_0 \alpha_1 | v | \alpha_0 \alpha_1 \rangle_{AS} = \langle \alpha_0 \alpha_1 | v | \alpha_0 \alpha_1 \rangle$$

$$- \langle \alpha_1 \alpha_0 | v | \alpha_0 \alpha_1 \rangle$$

$$\langle \alpha_0 \alpha_1 | v | \alpha_0 \alpha_1 \rangle_{AS} = \langle \alpha_1 \alpha_0 | v | \alpha_1 \alpha_0 \rangle_{AS}$$

$$\langle \alpha_0 \alpha_1 | v | \alpha_0 \alpha_1 \rangle_{AS} = - \langle \alpha_1 \alpha_0 | v | \alpha_0 \alpha_1 \rangle_{AS}$$

$$\int d\tau \; \Phi_0^* \, H_0 \, \Phi_0$$

$$\left(d\tau = d\vec{x}_1 \, d\vec{x}_2 \cdots d\vec{x}_N \right)$$

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

(i) $H_0 \hat{A}$

(ii) $\hat{A}^2 = A$ $\qquad \hat{A} = \dfrac{1}{N!} \sum_P (-)^p \hat{P}$

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

$$= \int \cdots \int d\vec{x}_1 \, d\vec{x}_2 \cdots d\vec{x}_N \; \varphi^*_{\alpha_0}(\vec{x}_1) \cdots \varphi^*_{\alpha_{N-1}}(\vec{x}_N)$$

$$\times \left(\hat{h}_0(\vec{x}_1) + \hat{h}_0(\vec{x}_2) + \cdots \hat{h}_0(\vec{x}_N) \right)$$

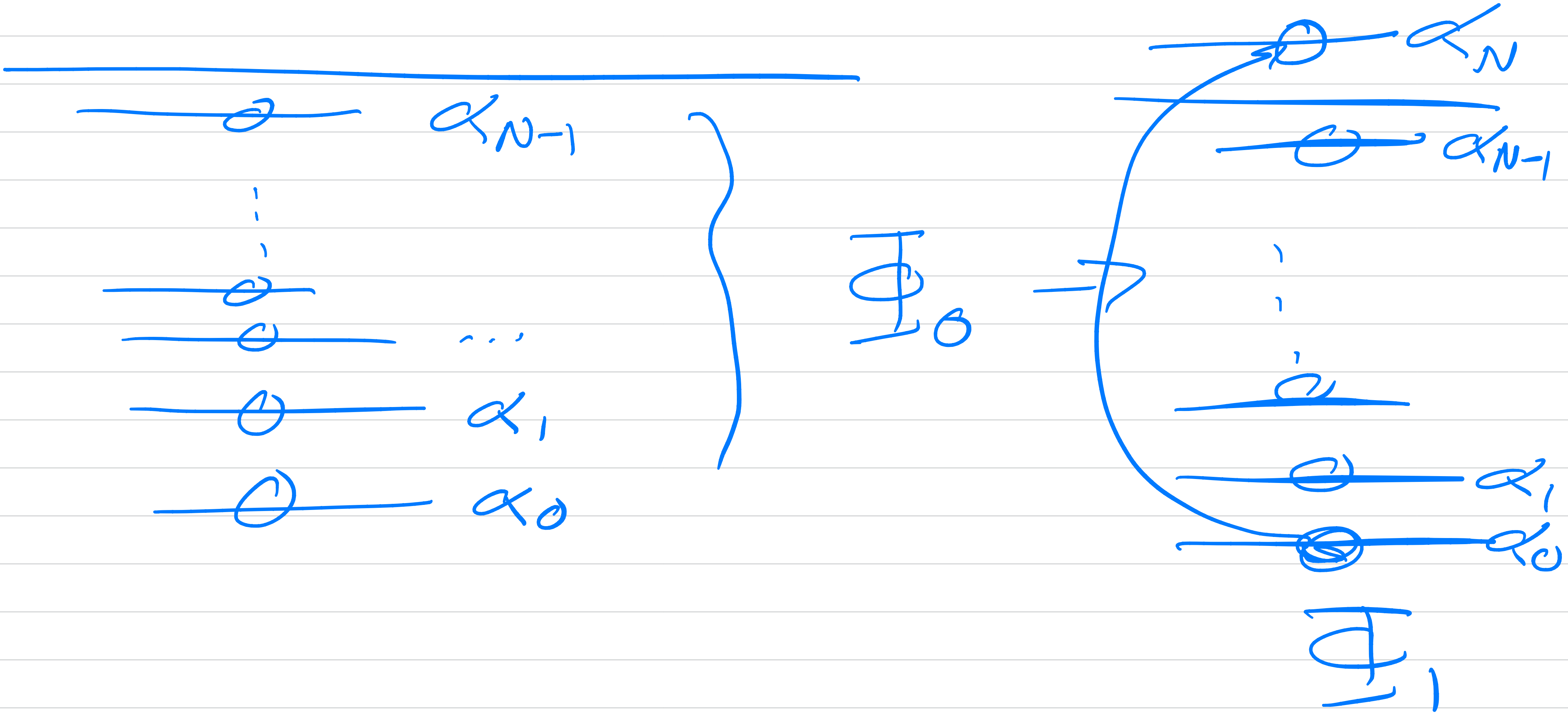
$$\times \sum_P (-1)^P \, \hat{P} \; \varphi_{\alpha_0}(\vec{x}_1) \varphi_{\alpha_1}(\vec{x}_2) \cdots \varphi_{\alpha_{N-1}}(\vec{x}_N)$$

$$h_0 \varphi_\alpha = \varepsilon_\alpha \varphi_\alpha$$

$P = 0$, no permutations

$\Rightarrow \sum_{\alpha_i} \varepsilon_{\alpha_i}$ $\qquad P \neq 0 \Rightarrow$ zero contrib.

$$\Phi_0 \to \Phi_1 : \quad \varphi_{\alpha_0}(\vec{x}_1) \to \varphi_{\alpha_N}(\vec{x}_1)$$



$$\langle \Phi_1 | H_0 | \Phi_0 \rangle$$

$$= \int \cdots \int dx_1\, dx_2 \cdots dx_N$$

ONB

$$\varphi^*_{\alpha_N}(\vec{x}_1)\, \varphi^*_{\alpha_{N+1}}(\vec{x}_2) \cdots \varphi^*_{\alpha_{N-1}}(\vec{x}_N)$$

$$\times \left(h_0(\vec{x}_1) + h_0(\vec{x}_2) \cdots h_0(\vec{x}_N) \right)$$

$$\sum_P (-)^P \hat{P}\, \varphi_{\alpha_0}(\vec{x}_1)\, \varphi_{\alpha_1}(\vec{x}_2) \cdots \varphi_{\alpha_{N-1}}(\vec{x}_N)$$

$$P = 0 \qquad \int \varphi^*_{\alpha_N}(x_1)\, h_0(x_1)\, \varphi_{\alpha_0}(x_1)$$

$\neq 0$ only if

φ_α not eigenbas

with onebody operator, we can have at most an SD which by one single-particle state in the bra and ket states,

$$\langle \Phi_i | H_0 | \Phi_j \rangle$$

if two or more differ then it is zero,

we have assumed an ONB single-particle basis.

two-body part

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle = \int d\tau\, \Phi_0^* H_I \Phi_0$$

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

(i) $\hat{H}_I \hat{A}$

(ii) $\hat{A}^2 = \hat{A}$

$$= \int d\tau\, \Phi_H^* \hat{H}_1 \sum_P (-)^P \hat{P}\, \varphi_{\alpha_0}(\vec{x}_1) \cdots \varphi_{\alpha_{N-1}}(\vec{x}_N)$$

$$= \sum_{i<j}^{N} \int d\vec{x}_1 \cdots d\vec{x}_N \, \varphi^*_{\alpha_0}(\vec{x}_1) \cdots \varphi^*_{\alpha_{N-1}}(\vec{x}_N)$$

$$v(x_i, x_j) \Big[1 - P_{ij} + O(P_{ij}^2) \Big]$$

$$P=0 \qquad P=1$$

$$\varphi_{\alpha_0}(\vec{x}_1)\, \varphi_{\alpha_1}(\vec{x}_2) \cdots \varphi_{\alpha_{N-1}}(\vec{x}_N)$$

$P=0$

$$\sum_{i<j}^{N} \int d\vec{x}_1 \cdots d\vec{x}_N \, \varphi^*_{\alpha_0}(\vec{x}_1) \cdots \varphi^*_{\alpha_{N-1}}(\vec{x}_N)$$

$$v(x_i, x_j)\, \varphi_{\alpha_0}(\vec{x}_1) \cdots$$

$$= \sum_{i<j} \langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle$$

$$P = 1$$

$$- \sum_{i<j} \int \dots dx_1' \quad \varphi^*_{\alpha_0}(x_1)\, \varphi^*_{\alpha_1} \dots \varphi^*_{\alpha_{N-1}}$$

$$v(x_i', x_j')\, \varphi_{\alpha_0}(x_1') \dots \underline{\varphi_{\alpha_i'}(x_j')}$$

$$\times \dots \underline{\varphi_{\alpha_j'}(x_i')} \dots \varphi_{\alpha_{N-1}}$$

$$= - \sum_{i<j} \langle \alpha_i \alpha_j | v | \alpha_j \alpha_i' \rangle$$