FYS4480/9480 lecture August 28, 2025

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

$$\hat{\mathcal{H}}_0 = \underbrace{\sum_{i=1}^{N} \hat{h}_0(x_i)}_{\text{onebody}}$$

$$\hat{h}_0(x_i) = -\frac{\hbar^2}{2m_i}\nabla_i^2 + V_{ext}(x_i)$$

$$x_i = (\vec{r}_i, \sigma_i)$$

$$\hat{h}_0(x_i)\varphi_{\alpha_j}(x_i) = \varepsilon_{\alpha_j}\varphi_{\alpha_j}(x_i)$$

$$\varphi_{\alpha_j}(x_i) = \psi_{\alpha_j}(\vec{r}_i) \otimes \xi_{\sigma_i}$$

$$\sigma_i = 1/2 \qquad m_{\sigma_i} = \begin{matrix} \uparrow \\ +1/2 \\ -1/2 \\ \downarrow \end{matrix}$$

$$\hat{H}_I = \sum_{i<j} v_2(x_i, x_j) + \sum_{i<j<k} v_3(x_i, x_j, x_k) + \ldots$$

$$\simeq \sum_{i<j} v(x_i, x_j)$$

$$v(x_i, x_j) \propto v'(|\vec{r}_i - \vec{r}_j|)$$

$$v(|\vec{r}_i-\vec{r}_j|) = v(r_{ij}) = \frac{\lambda}{|\vec{r}_i-\vec{r}_j|}$$

$$r_{ij} = |\vec{r}_i-\vec{r}_j| = \sqrt{(x_i-x_j)^2+(y_i-y_j)^2}$$

Slater determinant

$$\Phi_0(\vec{r}_1,\vec{r}_2 \ldots \vec{r}_N; \sigma_1,\sigma_2 \ldots \sigma_N; \alpha_1 \ldots \alpha_N)$$

$$(= \Phi_0(1,2, \ldots N))$$

$$=$$

$$\frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_1}(x_2) & \cdots & \varphi_{\alpha_1}(x_N) \\ \varphi_{\alpha_2}(x_1) & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ \varphi_{\alpha_N}(x_1) & \varphi_{\alpha_N}(x_2) & & \varphi_{\alpha_N}(x_N) \end{vmatrix}$$

$$\int dx\, \varphi^*_{\alpha_i}(x)\, \varphi_{\alpha_j}(x) = \delta_{\alpha_i \alpha_j}$$

$$= \langle \alpha_i | \alpha_j \rangle$$

Transposition

$$\hat{P}_{ij}\, \Phi(1,2,\ldots i \ldots j \ldots N)$$

$$= \Phi(1,2,\ldots j \ldots i \ldots N)$$

$$= - \Phi(1,2,\ldots i \ldots j \ldots N)$$

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11} a_{22} - a_{12} a_{21}$$

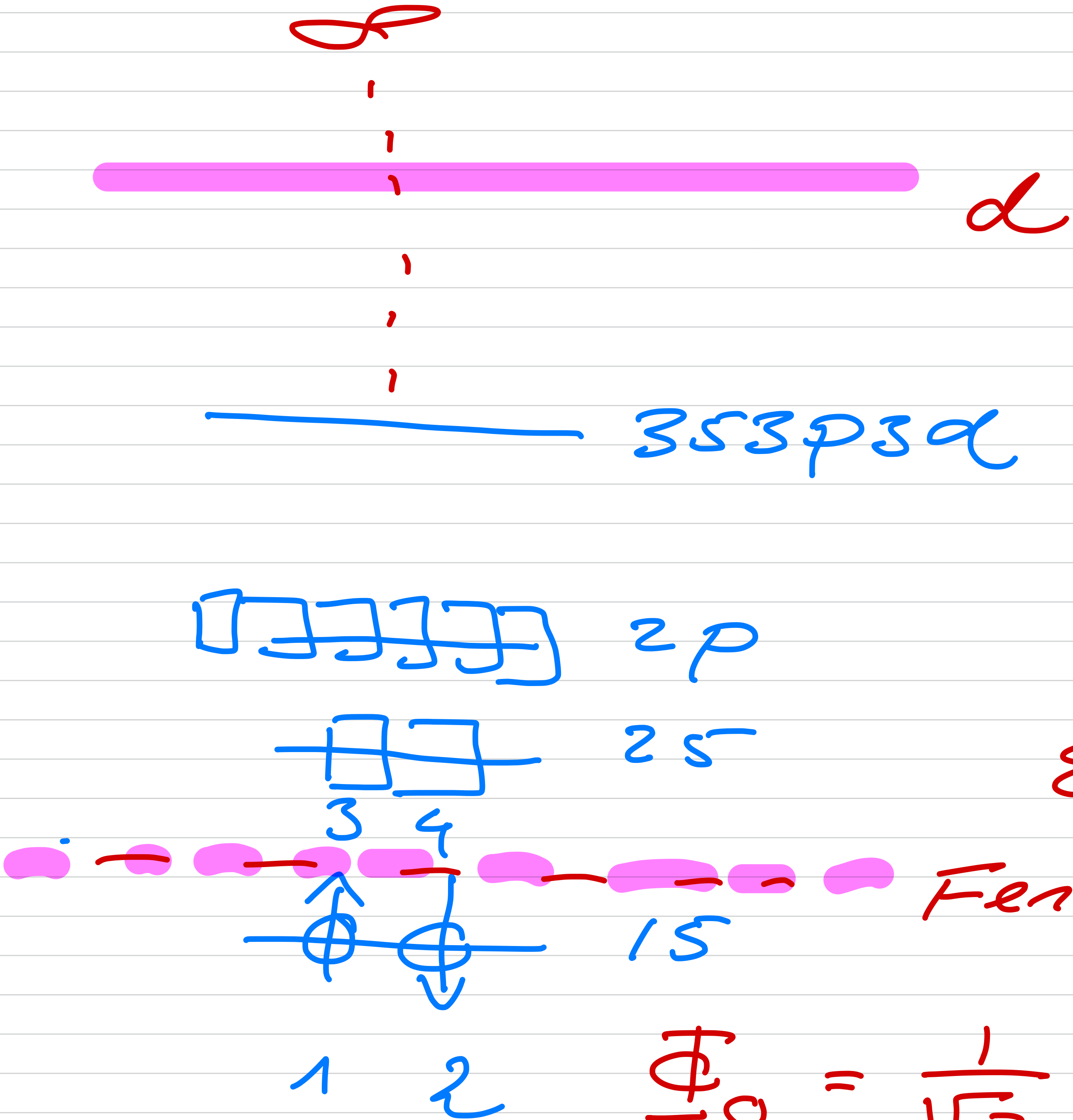
$$\det(A) = \sum_{\pi \in S_N} (-)^{\pi} \, a_{1\pi(1)} \, a_{2\pi(2)} \ldots a_{N\pi(N)}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \sum_{\pi \in S_N} (-)^{\pi} a_{1\pi(1)} a_{2\pi(2)} \times a_{3\pi(3)}$$

$$= a_{11} \left(a_{22} a_{33} - a_{32} a_{23} \right) + 4 \text{ more}$$

$$\underset{1\,2\,3}{\boxed{a_{11} a_{22} a_{33}}} - \underbrace{a_{11} a_{23} a_{32}}_{(1\,3\,2)}$$

$$+ (3\,2\,1) + (2\,1\,3) + \ldots$$



$\rightarrow n \geq N$

\# arrangements = configurations

$= n! / ((n-N)!\,N!)$

$$H_0 \Phi_0 = E_0 \Phi_0$$

$$E_0 = \varepsilon_{\alpha_1} + \varepsilon_{\alpha_2}$$

$$\Phi_0 = \frac{1}{\sqrt{2}} \left(\varphi_{\alpha_1}(x_1)\varphi_{\alpha_2}(x_2) - \varphi_{\alpha_1}(x_2)\varphi_{\alpha_2}(x_1) \right)$$

antisymmetrization operator

$$\hat{A} = \frac{1}{N!} \sum_{\pi \in S_N} (-)^{\pi} \hat{P}$$

idempotent

$$\hat{A}^2 = \hat{A} \quad ; \quad A^{+} = A$$

$N = 2$

$$\hat{A}_2 = \frac{1}{2}\left(1 - P_{12}\right)$$

$$\hat{A}_2^2 = \frac{1}{4}\left(1 - 2P_{12} + \underbrace{(P_{12})^2}_{1}\right)$$

$$= \frac{1}{2}\left(1 - P_{12}\right) = \hat{A}_2$$

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

$$= 0$$

$$\underline{\Phi}_0(1,2,\ldots N) = \sqrt{N!}\,\hat{A}\,\underbrace{\underline{\Phi}_H(12\ldots N)}$$

Hartree function

$$\underline{\Phi}_H(1,2\ldots N) = \varphi_{\alpha_1}(x_1)\,\varphi_{\alpha_2}(x_2)\ldots$$

$$\varphi_{\alpha_N}(x_N)$$

$$(a_{11}\, a_{22}\, a_{33} \ldots)$$

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

$$\hat{\mathcal{H}} \Phi_0 \neq E_0 \Phi_0$$

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

$$= \frac{\langle \Phi_0 | \mathcal{H}_0 | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}$$

$$= \underline{1}$$

$$d\vec{\tau} = dx_1 dx_2 \dots dx_N$$

$$\int dx = \sum_{\sigma} \int d\vec{r}$$

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

$$= \int d\tau \, \Phi_0^*(1,2,\ldots N) \, \hat{H}_0 \, \Phi_0(1,2,\ldots N)$$

$$= N! \int d\tau \, \underline{\Phi}_H^* \hat{A} \underbrace{\left(\sum_{i=1}^{N} \hat{h}_0(x_i)\right)}_{\hat{H}_0} \hat{A} \, \underline{\Phi}_H$$

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

$$\hat{A}^2 = \hat{A}$$

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

$$= \int d\tilde{r}\, \Phi_H^* \hat{H}_0 \sum_{\pi \in S_N} (-)^\pi \hat{P}\, \Phi_H$$

(i) zero permutations

$$\int dx_1 \int dx_2 \cdots \int dx_N\, \varphi^*_{\alpha_1}(x_1)\, \varphi^*_{\alpha_2}(x_2) \cdots \varphi^*_{\alpha_N}(x_N) \left(\hat{h}_0(x_1) + \hat{h}_0(x_2) + \cdots \hat{h}_0(x_N) \right)$$

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

$$= \int dx_1\, \varphi^*_{\alpha_1}(x_1)\, \underbrace{\hat{h}_0(x_1)\, \varphi_{\alpha_1}(x_1)}_{\varepsilon_{\alpha_1} \varphi_{\alpha_1}(x_1)} \int dx_2\, \varphi^*_{\alpha_2}(x_2)\, \varphi_{\alpha_2}(x_2) \cdots \int dx_N\, \varphi^*_{\alpha_N}(x_N)\, \varphi_{\alpha_N}(x_N)$$

$$= \boxed{\sum_{i=1}^{N} \varepsilon_{\alpha_i}}$$

1-permutations $1 \leftrightarrow 2$

$$\int dx_1 \int dx_2 \ldots \int dx_N$$

$$\varphi_{\alpha_1}^*(x_1)\, \varphi_{\alpha_2}^*(x_2) \ldots \varphi_{\alpha_N}^*(x_N)$$

$$\left(\hat{h}_0(x_1) + \hat{h}_0(x_2) + \ldots + \hat{h}_0(x_N) \right)$$

$$\varphi_{\alpha_1}(x_2)\, \varphi_{\alpha_2}(x_1) \ldots \varphi_{\alpha_N}(x_N)$$

$= 0$ + all other permutations –

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

$$= N! \int d\vec{r}\ \Phi_H^* \hat{A}^\dagger \hat{\mathcal{H}}_I \hat{A}\, \Phi_H$$

$$[\hat{\mathcal{H}}_I, \hat{A}] = \hat{\mathcal{H}}_I \hat{A} - \hat{A}\hat{\mathcal{H}}_I = 0$$

$$= N! \int d\vec{r}\ \Phi_H^* \hat{\mathcal{H}}_I \hat{A}\, \Phi_H$$

$$= \int d\vec{r}\ \Phi_H^* \hat{\mathcal{H}}_I \sum_{\pi \in S_N} (-)^\pi \hat{P}\, \Phi_H =$$

$$\sum_{i<j} \int dx_1 \ldots dx_i' \ldots dx_j' \ldots dx_N$$

$$\varphi^*_{\alpha_1}(x_1)\,\varphi^*_{\alpha_2}(x_2)\ldots\varphi^*_{\alpha_i}(x_i)\ldots\varphi^*_{\alpha_j}(x_j)\ldots$$

$$\varphi^*_{\alpha_N}(x_N)\; v(x_i', x_j') \sum_{P\in S_N} (-)^{\pi}\, \hat{P}$$

$$\varphi_{\alpha_1}(x_1)\ldots\varphi_{\alpha_i}(x_i')\ldots\varphi_{\alpha_j}(x_j')\ldots\varphi_{\alpha_N}(x_N)$$

$P = 0$ no permutations

and x_i' and x_j'

$$\sum_{i<j} \int dx_i \int dx_j \; \varphi^*_{\alpha_i}(x_i)\, \varphi^*_{\alpha_j}(x_j)$$

$$\underbrace{\times \; v(x_i, x_j)\, \varphi_{\alpha_i}(x_i)\, \varphi_{\alpha_j}(x_j)}_{\langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle}$$

Direct term

$P = 1 \qquad (i \Longleftrightarrow j)$

$$- \sum_{i<j} \int dx_i \int dx_j \; \varphi^*_{\alpha_i}(x_i)\, \varphi^*_{\alpha_j}(x_j)$$

$$\times \; v(x_i, x_j)\, \varphi_{\alpha_i}(x_j)\, \varphi_{\alpha_j}(x_i)$$

Exchange term $\quad \langle \alpha_i \alpha_j | v | \alpha_j \alpha_i \rangle$

All other permutations are zero

$$\langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \underbrace{\sum_{i=1}^{N} \underbrace{\langle \alpha_i | \hat{h}_0 | \alpha_i \rangle}_{\varepsilon_{\alpha_i}}}_{\varepsilon_0} + \frac{1}{2} \sum_{\alpha_i \alpha_j} \left(\langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle - \langle \alpha_i \alpha_j | v | \alpha_j \alpha_i \rangle \right)$$

$$\hat{h}_0 \Phi_0 = \varepsilon_0 \Phi_0$$

$$\langle ij|v|ke\rangle_{AS} = \langle ij|v|ke\rangle - \langle ij|v|ek\rangle$$

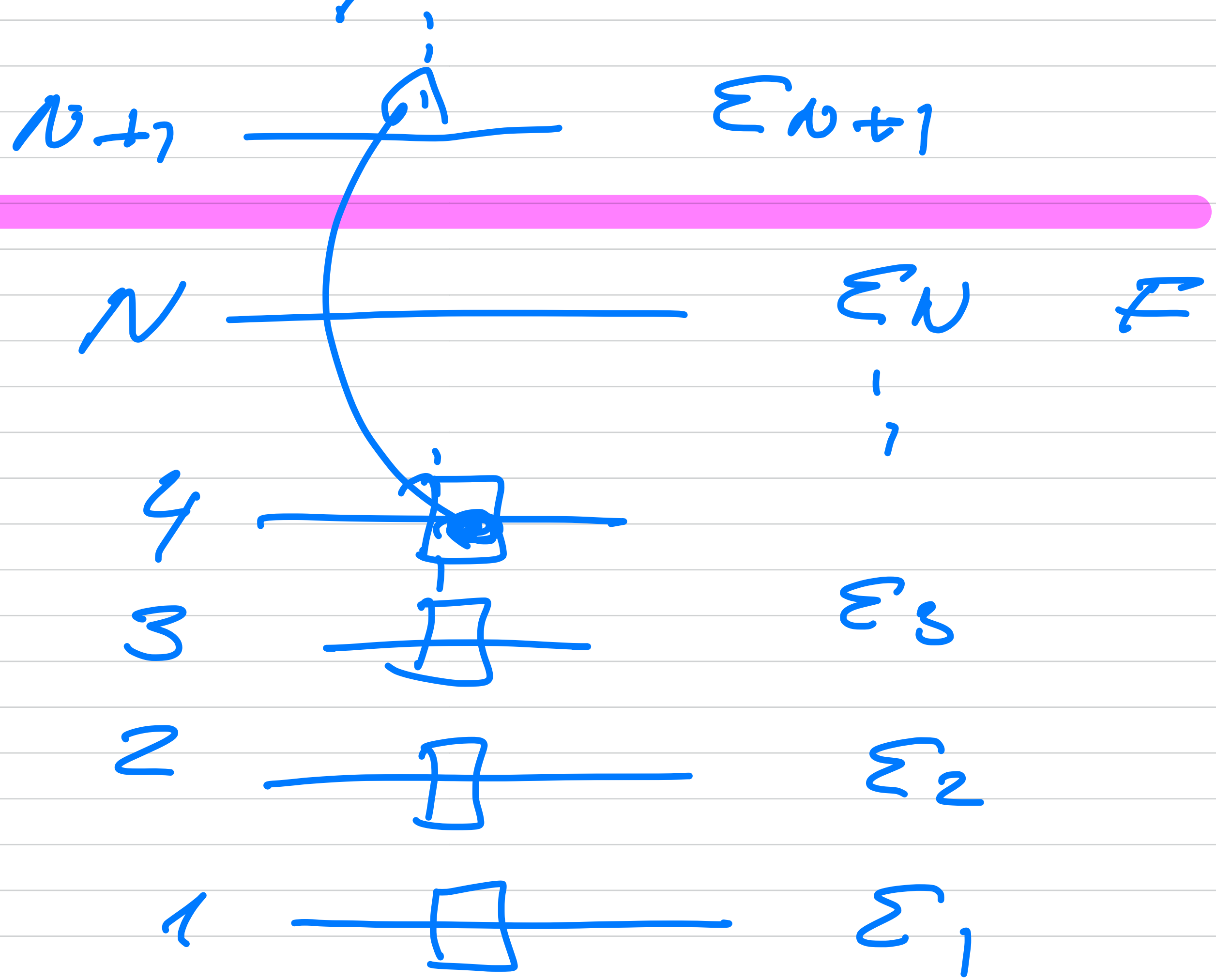
$$\langle ij|v|ke\rangle_{AS} = \langle ji|v|ek\rangle_{AS}$$

$$= -\langle ji|v|ke\rangle_{AS}$$

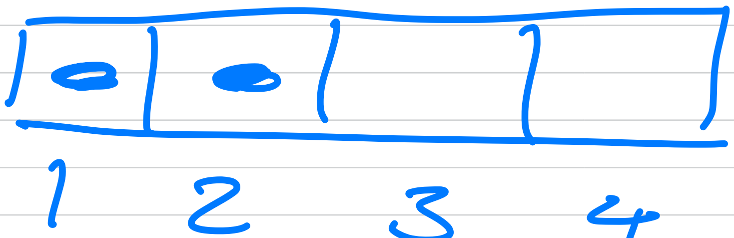
$$\langle \Phi_0 | \mathcal{H}^? | \Phi_0 \rangle$$

$$= \varepsilon_0 + \frac{1}{2}\sum_{ij} \langle ij|v|ij\rangle_{AS}$$

Number representation
(2nd quantization)

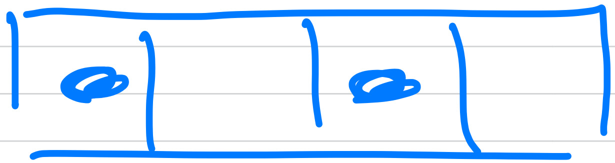


$N = 2 \qquad n = 4 \qquad \# \; \frac{4!}{2!\,2!} = 6$



$\rightarrow 1100$

$|1100\rangle$



$\rightarrow 1010$

$|1010\rangle$

Vacuum $|0\rangle$