Lecture FYS4480/9480, August 29, 2024

FYS4480/9480 AUGUST 29

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

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}_0(x_i) \qquad x_i = (\vec{r}_i, \sigma_i)$$

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

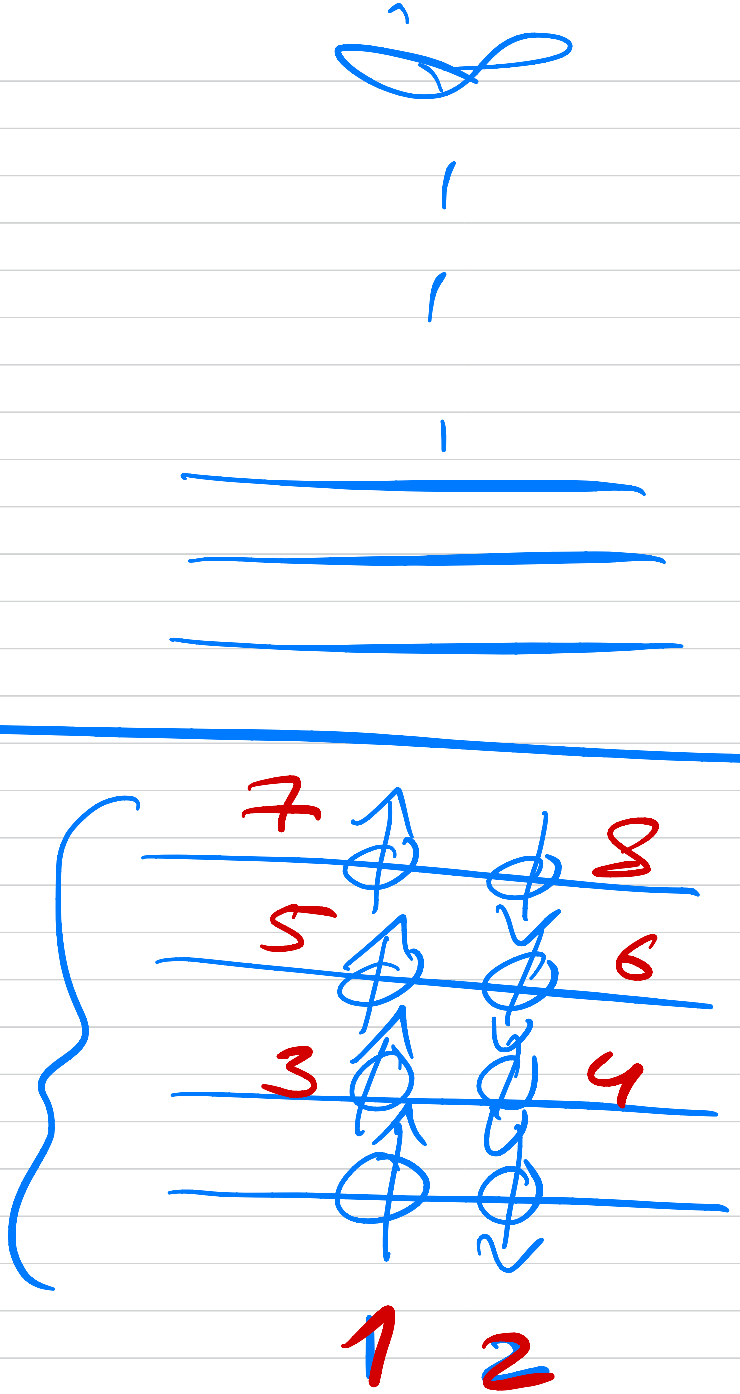
1-dim, HO $\quad \hat{h}_0(x_i) = -\frac{\hbar^2}{2m}\frac{d^2}{dx_i^2} + \frac{1}{2}k x_i^2$

no-spin dependence

$$\varphi_\alpha(x_i) = \Phi_\alpha(x_i) \otimes \xi_{\sigma_\alpha}$$

$$E_\alpha = \hbar\omega\left(n_\alpha + \tfrac{1}{2}\right)$$

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



$\alpha = 4$

Φ_0

$\alpha = 3$

$\alpha = 2$

$\alpha = 1$

$\alpha = 0$

Fermi level

$N = 8$

lowest-lying state for N particles

$$\Phi_0(x_1 x_2 \ldots x_N; \alpha_0 \alpha_1 \ldots \alpha_{N-1})$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_0}(x_1) & \varphi_{\alpha_0}(x_2) & \ldots & \varphi_{\alpha_0}(x_N) \\ \varphi_{\alpha_1}(x_1) & & & \\ \vdots & & & \\ \varphi_{\alpha_{N-1}}(x_1) & - & - & \varphi_{\alpha_{N-1}}(x_N) \end{vmatrix}$$

$$= \frac{1}{\sqrt{N!}} \sum_{P=0}^{P!} (-)^P \hat{P} \, \Phi_H(x_1 x_2 \ldots; \alpha_0 \ldots)$$

$$\Phi_H = \varphi_{\alpha_0}(x_1)\,\varphi_{\alpha_1}(x_2) \cdots \varphi_{\alpha_{N-1}}(x_N)$$

Hartree-function

$$[\hat{H}, \hat{P}] = 0$$

Antisymm rerator

$$\hat{A} = \frac{1}{N!} \sum_{P}^{P!} (-)^{P} \hat{P} \; ; \; [\hat{A}, \hat{H}], \hat{A}^2 = \hat{A}$$

$N = 2$

$$\hat{A} = \frac{1}{2}\Big(\underbrace{\hat{P}_{12}}_{}^{P=0} - \hat{P}_{21}\Big)$$

$$\hat{A}_2^2 = \frac{1}{4}\Big(1 - 2\hat{P}_{21} + \hat{P}_{21}^{2}\Big)^{1} = \frac{1}{2}\big(1 - \hat{P}_{21}\big)$$

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11} a_{22} - \underbrace{a_{12} a_{21}}_{2 \leftrightarrow 1}$$

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

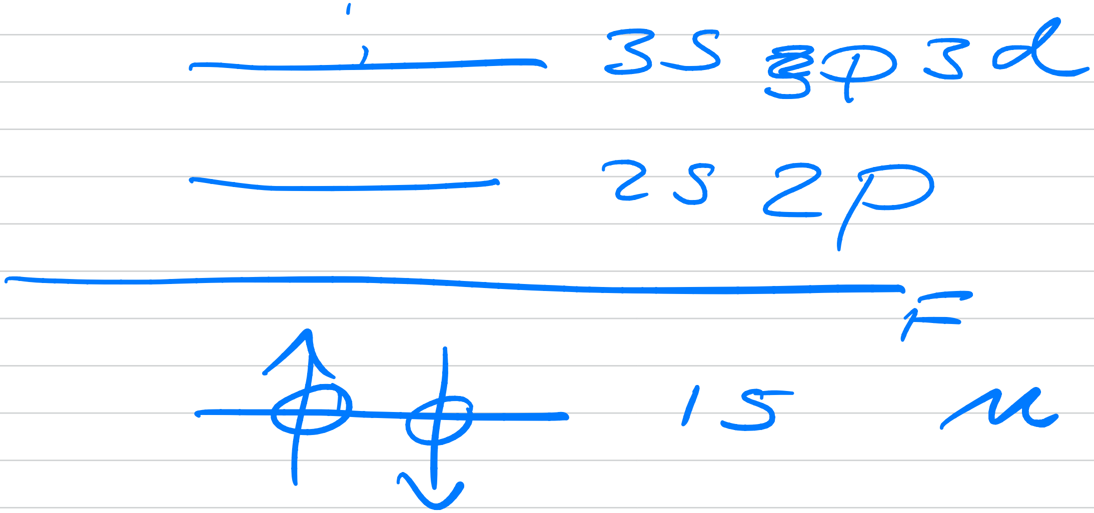
$$= a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix}$$

$$\underset{1}{+} \; a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$

$$= P_{123} - P_{132} + P_{312} - P_{213} + P_{231} - P_{321}$$

$$\Phi_0 = \sqrt{N!}\,\hat{A}\,\Phi_H$$

Example: Atomic Helium



$n=0,\ l=0,\ m_l=0$

$$E = -\frac{E_0}{n^2}$$

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

$$\Phi_0 = \frac{1}{\sqrt{2!}} \begin{vmatrix} \varphi_{\alpha_0}(x_1) & \varphi_{\alpha_0}(x_2) \\ \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_1}(x_2) \end{vmatrix}$$

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

$$= \frac{1}{2} \sum_{i=1}^{2} \int dx_1 \int dx_2 \left[\varphi^*_{\alpha_0}(x_1) \varphi^*_{\alpha_1}(x_2) - \varphi^*_{\alpha_0}(x_2) \varphi^*_{\alpha_1}(x_1) \right] \hat{h}_0(x_i)$$
$$\times \left[\varphi_{\alpha_0}(x_1) \varphi_{\alpha_1}(x_2) - \varphi_{\alpha_0}(x_2) \varphi_{\alpha_1}(x_1) \right]$$

$h_0(x_1)$:

E_{α_0} $\qquad\qquad E_{\alpha_0}\varphi_{\alpha_0}(x_1)$

$$\int dx_1\, dx_2 \Big[\varphi^*_{\alpha_0}(x_1) \boxed{\hat{h}_0(x_1)\, \varphi_{\alpha_0}(x_1)} \times \varphi^*_{\alpha_1}(x_2)\, \varphi_{\alpha_1}(x_2)$$

0 $\qquad\qquad E_{\alpha_0}\varphi_{\alpha_0}(x_1)$

$$- \varphi^*_{\alpha_0}(x_2)\, \varphi^*_{\alpha_1}(x_1) \boxed{\hat{h}_0(x_1)\, \varphi_{\alpha_0}(x_1)}\, \varphi_{\alpha_1}(x_2)$$

$$E_{\alpha_1} \quad + \varphi^*_{\alpha_0}(x_2)\, \underline{\varphi^*_{\alpha_1}(x_1)}\, \hat{h}_0(x_1)\, \varphi_{\alpha_0}(x_2)\, \varphi_{\alpha_1}(x_1)$$

0 $\qquad\qquad \underline{E_{\alpha_1}\varphi_{\alpha_1}(x_1)}$

$$- \varphi^*_{\alpha_0}(x_1)\, \varphi^*_{\alpha_1}(x_2)\, h_0(x_1)\, \varphi_{\alpha_0}(x_2)\, \varphi_{\alpha_1}(x_1) \Big]$$

$$h_0(x_1) \quad : \quad \frac{1}{2}\left(\varepsilon_{\alpha_0} + \varepsilon_{\alpha_1}\right)$$

$$h_0(x_2) \quad : \quad \frac{1}{2}\left(\varepsilon_{\alpha_0} + \varepsilon_{\alpha_1}\right)$$

$$\hat{H}_0 \Phi_0 = \mathcal{E}_0 \Phi_0$$

$$\mathcal{E}_0 = \sum_{\alpha_i} \varepsilon_{\alpha_i}$$

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

$$\hat{H}_I = \sum_{i<j}^{N} v(r_{ij})$$

$$r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

$$r_{ij}' = r_{ji}$$

$$\frac{1}{2} \int dx_1\, dx_2 \left[\varphi_{\alpha_0}^*(x_1)\, \varphi_{\alpha_1}^*(x_2) - \varphi_{\alpha_0}^*(x_2)\, \varphi_{\alpha_1}^*(x_1) \right]$$

$$\times \quad v(r_{12}) \Big[\varphi_{\alpha_0}(x_1)\, \varphi_{\alpha_1}(x_2)$$

$$- \varphi_{\alpha_0}(x_2)\, \varphi_{\alpha_1}(x_1) \Big]$$

$$\frac{1}{2}\int dx_1 dx_2\; \varphi^*_{\alpha_0}(x_1)\,\varphi^*_{\alpha_1}(x_2)\,v(r_{12})\,\varphi_{\alpha_0}(x_1)\,\varphi_{\alpha_1}(x_2)$$

$$+\frac{1}{2}\int dx_1 dx_2\; \varphi^*_{\alpha_0}(x_2)\,\varphi^*_{\alpha_1}(x_1)\,v(r_{12})\,\varphi_{\alpha_0}(x_2)\,\varphi_{\alpha_1}(x_1)$$

$$x_1 \leftrightarrow x_2$$

$$-\frac{1}{2}\int dx_1 dx_2\; \varphi^*_{\alpha_0}(x_2)\,\varphi^*_{\alpha_1}(x_1)\,v(r_{12})\,\varphi_{\alpha_0}(x_1)\,\varphi_{\alpha_1}(x_2)$$

$$-\frac{1}{2}\;\text{——}\;''\;\text{——}\;\varphi^*_{\alpha_0}(x_1)\,\varphi^*_{\alpha_1}(x_2)\,v(r_{12})\,\varphi_{\alpha_0}(x_2)\,\varphi_{\alpha_1}(x_1)$$

$$x_1 \leftrightarrow x_2$$

short hand

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

$$= \int dx_1 dx_2 \, \varphi^*_{\alpha_0}(x_1) \varphi^*_{\alpha_1}(x_2) \, v(r_{12})$$

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

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

$$\Rightarrow \quad \langle \Phi_0 | H_1 | \Phi_0 \rangle =$$

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

$$\langle pq | v | rs \rangle_{AS} = \langle pq | v | rs \rangle - \langle pq | v | sr \rangle$$

$$\langle pq | v | rs \rangle_{AS} = \langle qp | v | sr \rangle_{AS}$$

$$\langle pq | v | rs \rangle_{AS} = - \langle qp | v | rs \rangle_{AS}$$

$$\langle - \quad | - \rangle_{AS} = - \langle pq | v | sr \rangle_{AS}$$

$$\langle \Phi_0 | H | \Phi_0 \rangle = \varepsilon_{\alpha_0} + \varepsilon_{\alpha_1} + \langle \alpha_0 \alpha_1 | v | \alpha_0 \alpha_1 \rangle_{AS}$$

N-particles

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \int dx_1\, dx_2 \ldots dx_N \times \Phi_0^* \hat{H}_0 \Phi_0$$

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

$$\int dx_1 \int dx_2 \int \cdots \int dx_N = \int d\tau$$

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle =$$

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

$$(i) \quad [\hat{A}, \hat{H}_0] = 0$$

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

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

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

$P = 0$

$$\sum_{i=1}^{N} \int dx_1 dx_2 \cdots dx_N \, \varphi^*_{\alpha_0}(x_1) \cdots \varphi^*_{\alpha_{N-1}}(x_N)$$

$$\times \hat{h}_0(x_i) \, \varphi_{\alpha_0}(x_1) \varphi_{\alpha_1}(x_2) \cdots \varphi_{\alpha_{N-1}}(x_N)$$

$$= \sum_{\alpha_i' = \alpha_0}^{\alpha_{N-1}} \varepsilon_{\alpha_i'}$$

$P = 1$ (one example)

$$\sum_{i=1}^{N} \int dx_1 dx_2 \cdots dx_N \, \varphi^*_{\alpha_0}(x_1) \cdots \varphi^*_{\alpha_{N-1}}(x_N)$$

$$\times h_0(x_i) \, \varphi_{\alpha_0}(x_2) \varphi_{\alpha_1}(x_1) \cdots$$

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

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

(i) $[\hat{H}_I, \hat{A}] = 0$

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

$$= \int d\tau \, \phi_H^* H_I \sum_p^{p!} (-)^p \hat{P} \Phi_H$$

$$= \frac{1}{2} \sum_{\alpha_i \alpha_j} \langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle_{AS}$$