FYS 4480 AUGUST 26

$$\hat{h}_0 \varphi_i(\vec{r}) = \varepsilon_i \varphi_i(\vec{r})$$

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

— Additional compact notation

$$\vec{x} = (\vec{r}, s)$$

$$\varphi(\vec{r}) \otimes \xi_{s m_s} = |\vec{r} s m_s\rangle$$

$$= |\vec{x}\rangle \quad (|x\rangle)$$

$$\int dx = \sum_{m_s = \pm 1/2} \int d\vec{r}$$

$$s = 1/2$$

$$\delta(x - x') = \delta_{m_s m_s'} \delta^{(d)}(\vec{r} - \vec{r}')$$

$$\langle x | x' \rangle = \delta(x - x')$$

sp states $\quad \varphi_i(\vec{r}_j)$

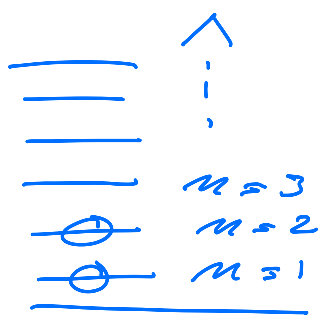
particle j

Fermions $(N=2)$, ansatz for $\Phi(\vec{r}_1, \vec{r}_2)$

$$= \frac{1}{\sqrt{2!}} \begin{vmatrix} \varphi_\alpha(\vec{r}_1) & \varphi_\alpha(\vec{r}_2) \\ \varphi_\beta(\vec{r}_1) & \varphi_\beta(\vec{r}_2) \end{vmatrix}$$

$$\Phi(\vec{r}_1, \vec{r}_2) = - \Phi(\vec{r}_2, \vec{r}_1)$$

$$\Phi(\vec{r}_1, \vec{r}_2) = \Phi$$



$$h_0 |1\rangle = \varepsilon_1 |1\rangle$$

$$h_0 |i\rangle = \varepsilon_i |i\rangle$$

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

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

$$|\Phi_0\rangle = |12\rangle$$

Direct

$$= \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \int d\vec{r}_1 \, d\vec{r}_2 \Big(\varphi_1^*(\vec{r}_1) \varphi_2^*(\vec{r}_2) - \varphi_1^*(\vec{r}_2) \varphi_2^*(\vec{r}_1) \Big)$$

$$\times \left(\hat{h}_0(\vec{r}_1) + h_0(\vec{r}_2) \right)$$

$$\times \left(\varphi_1^*(\vec{r}_1)\, \varphi_2(\vec{r}_2) - \varphi_1(\vec{r}_2)\, \varphi_2(\vec{r}_1) \right)$$

$$= \frac{1}{2} \Bigg(\overbrace{\int d\vec{r}_2\, \varphi_2^*(\vec{r}_2)\, \varphi_2(\vec{r}_2)}^{=1} \underbrace{\int d\vec{r}_1\, \varphi_1^*(\vec{r}_1)\, \hat{h}_0\, \varphi_1(\vec{r}_1)}_{\varepsilon_1}$$

$$- \underbrace{\int d\vec{r}_2\, \varphi_2^*(\vec{r}_2)\, \varphi_1(\vec{r}_2)}_{=0} \int d\vec{r}_1 \ldots$$

$$+ \frac{1}{2} \qquad + 0$$

$$- \underbrace{\int d\vec{r}_2\, \varphi_1^*(\vec{r}_2)\, \varphi_2(\vec{r}_2)}_{=0} \int d\vec{r}_1 \ldots$$

$$+ \varepsilon_2$$

$$+ 0 + \varepsilon_1$$

$$= \varepsilon_1 + \varepsilon_2$$

$$\Phi_0(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$$

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \sum_{i=1} \varepsilon_i$$

$$= \mathcal{E}_0$$

$$\varepsilon_i = \int d\vec{r}\, \varphi_i^*(\vec{r})\, \hat{h}_0(\vec{r})\, \varphi_i(\vec{r})$$

$$= \langle i | \hat{h}_0 | i \rangle$$

$$= \langle i | h_0 | i \rangle$$

$$\langle j | h_0 | i \rangle = \delta_{ij}\, \varepsilon_i$$

$$H_I = \sum_{i<j} v(r_{ij})$$

$$\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$$

$$r_{ij} = |\vec{r}_{ij}|$$

$$= \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + \ldots}$$

$$\langle \Phi_0 | \hat{H}_1 | \Phi_0 \rangle =$$

$$\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \int d\vec{r}_1\, d\vec{r}_2 \left(\varphi_1^*(\vec{r}_1) \right) \varphi_2^*(\vec{r}_2)$$

$$- \varphi_1^*(\vec{r}_2)\varphi_2^*(\vec{r}_1)\Big)\, v(r_{12})$$

$$\times \left(\varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2) - \varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1)\right)$$

$$+ \frac{1}{2}\int d\underline{\vec{r}_1}\, d\underline{\vec{r}_2} \Big\{$$

$$\varphi_1^*(\vec{r}_1)\varphi_2^*(\vec{r}_2)\, v(r_{12})\, \varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2)$$

$$+ \varphi_1^*\underset{\vec{r}_1}{(\vec{r}_2)}\overset{\vec{r}_2}{\varphi_2^*(\vec{r}_1)}\, v(r_{12})\, \varphi_1\underset{\vec{r}_1}{(\vec{r}_2)}\varphi_2\underset{\vec{r}_2}{(\vec{r}_1)}\Big)$$

$$\vec{r}_1 \leftrightarrow \vec{r}_2$$

$$- \frac{1}{2}\int d\vec{r}_1\, d\vec{r}_2 \Big\{ \varphi_1^*(\vec{r}_2)\varphi_1(\vec{r}_1)$$

$$\times v(r_{12})\, \varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2)$$

$$+ \varphi_1^*(\vec{r}_1)\varphi_2(\vec{r}_2)\, v(r_{12})$$

$$\varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1) \Big\}$$

$$= \int d\vec{r}_1 d\vec{r}_2 \, \varphi_1^*(\vec{r}_1) \varphi_2^*(\vec{r}_2) v(r_{12}) \times \varphi_1(\vec{r}_1) \varphi_2(\vec{r}_2)$$

Direct term

$\langle 12 | v | 12 \rangle$

$$- \int d\vec{r}_1 d\vec{r}_2 \, \varphi_1^*(\vec{r}_2) \varphi_2^*(\vec{r}_1) \times v(r_{12}) \varphi_1(\vec{r}_1) \varphi_2(\vec{r}_2)$$

Exchange term

$\langle 21 | v | 12 \rangle$

$$\langle 12 | v | 12 \rangle - \langle 21 | v | 12 \rangle$$

$$\underset{100^2}{\langle pq | v | pq \rangle} - \underset{100^2}{\langle qp | v | pq \rangle}$$

$$= \langle pq | v | pq \rangle_{AS}$$

N-body SD

$$\Phi_0(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N; \alpha_1, \alpha_2 \dots \alpha_N)$$

$$| \varphi_1(\vec{r}_1) \dots \varphi_N(\vec{r}_N) |$$

$$
= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_1}(\vec{r}_1) & \cdots & \varphi_{\alpha_1}(\vec{r}_N) \\ \varphi_{\alpha_2}(\vec{r}_1) & & \vdots \\ \vdots & & \vdots \\ \varphi_{\alpha_N}(\vec{r}_1) & & \varphi_{\alpha_N}(\vec{r}_N) \end{vmatrix}
$$

$$
= \frac{1}{\sqrt{N!}} \sum_P (-)^P \hat{P}\, \varphi_{\alpha_1}(\vec{r}_1) \cdots \varphi_{\alpha_N}(\vec{r}_N)
$$

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

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

$$
\Phi_H = \varphi_{\alpha_1}(\vec{r}_1)\, \varphi_{\alpha_2}(\vec{r}_2) \cdots \varphi_{\alpha_N}(\vec{r}_N)
$$