One Body Hamiltonian

Coulomb interaction does not change spin

spin is conserved

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

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

magnetic field Hamiltonian change spin of particle

Additional Compact Notations:

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

(contain spatial dof, spin).

$$\psi(\vec{r}_i) \otimes \xi_{s, m_s} = |\vec{r}, s\, m_s\rangle$$

$$= |x\rangle \quad (|x\rangle)$$

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

1D

2D

3D

$s = 1/2$

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

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

single particle state $\quad \phi_i(x_j)$

particle j with quantum # i

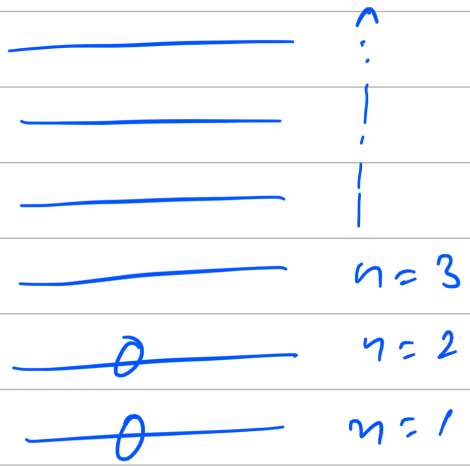
Fermions $(N=2)$; ansatz

for $$\Phi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_\alpha(r_1) & \phi_\alpha(r_2) \\ \phi_\beta(\vec{r}_1) & \phi_\beta(\vec{r}_2) \end{vmatrix}$$

for two particle system:

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

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



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

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

Solve this by brute force:

$$\varepsilon_1 < \varepsilon_2 < \cdots\cdots$$

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

$|\Phi_0\rangle = |12\rangle$ Tensor product of $\underline{1 \& 2}$

Direct Term

$$\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \int d\vec{r}_1 \, d\vec{r}_2 \left(\Phi_1^*(\vec{r}_1) \Phi_2^*(\vec{r}_2) - \Phi_1^*(\vec{r}_2) \Phi_2^*(\vec{r}_1) \right) \times$$

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

$$\left[\Phi_1(\vec{r}_1) \Phi_2(\vec{r}_2) - \Phi_1(\vec{r}_2) \Phi_2(\vec{r}_1) \right]$$

$$= \frac{1}{2} \Big(\underbrace{\int d\vec{r}_2 \, \Phi_2^*(\vec{r}_2) \Phi_2(\vec{r}_2)}_{=1} \underbrace{\int d\vec{r}_1 \, \Phi_1^*(r_1) \cdot \hat{h}_0 \Phi_1(r_1)}_{\varepsilon_1}$$

$$- \underbrace{\int d\vec{r}_2 \, \Phi_2^*(r_2) \Phi_1(r_2) \int d\vec{r}_1}_{=0}$$

$$+ \frac{1}{2} + 0 - \underbrace{\int d\vec{r}_2 \, \Phi_1^*(r_2) \Phi_2(\vec{r}_2) \int d\vec{r}_1}_{=0} \cdots\cdots$$

$$+ \varepsilon_2 + 0 + \varepsilon_1$$

$= \mathcal{E}_1 + \mathcal{E}_2$

for single particle state :-

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

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \sum_{i=1}^{N} \mathcal{E}_i = \mathcal{E}_0$$

$$\mathcal{E}_i = \int d\vec{r}_i \, \phi_i^*(\vec{r}) \, \hat{h}_0(\vec{r}_i) \, \phi_i(\vec{r})$$

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

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

Now look at the interaction part :-

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

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

$$r_{ij} = |\vec{r}_{ij}| = \sqrt{(x_i - x_j)^2 + \cdots\cdots}$$

$$\langle \Phi_0 | H_I | \Phi_0 \rangle = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \int d\vec{r}_1 d\vec{r}_2 \left(\phi_1^*(\vec{r}_1) \phi_2^*(\vec{r}_2) - \phi_1^*(\vec{r}_2) \cdot \phi_2^*(\vec{r}_1) \right)$$

1 2

$$v(r_{12}) \times \left[\left(\phi_1(\vec{r}_1) \phi_2(\vec{r}_2) - \phi_1(\vec{r}_2) \phi_2(\vec{r}_1) \right) \right]$$

3 4 5

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

1 3 4 $\Rightarrow$

$$+\frac{1}{2}\int d\vec{r}_1\, d\vec{r}_2 \Big\{ \phi_1^*(\vec{r}_1)\,\phi_2^*(r_2)\,v(r_{12})\,\phi_1(r_{12})\,\phi_2(r_2) \; +$$

$$\phi_1^*(r_2)\,\phi_2^*(r_1)\,v(r_{12})\,\phi_1(\vec{r}_2)\,\phi_2(\vec{r}_1) \Big\}$$

If we change $\vec{r}_1 \leftrightarrow \vec{r}_2$

There is no evidence of breaking of symmetry of relative distance betn the particle.

$\downarrow$

Translational symmetry

$$= \frac{1}{2}\int d\vec{r}_1\, d\vec{r}_2 \Big\{ \phi_1^*(r_2)\,\phi_1(\vec{r}_1) \times v(r_{12}) \times \phi_1(r_1)\,\phi_2(r_2)$$

$$+\; \phi_1^*(r_1)\,\phi_2(\vec{r}_2)\,v(r_{12})\,\phi_1(\vec{r}_2)\,\phi_2(\vec{r}_1) \Big\}$$

$$= \int \underbrace{d\vec{r}_1\, d\vec{r}_2\; \phi_1^*(r_1)\,\phi_2(\vec{r}_2)\,v(r_{12})\,\phi_1(\vec{r}_1)\,\phi_2(\vec{r}_2)}_{\text{Direct Term.}}$$

$$\langle 12|v|12\rangle$$

$$- \int d\vec{r}_1 \, d\vec{r}_2 \, \phi_1^*(\vec{r}_2) \, \phi_2(\vec{r}_1) \times v(r_1, r_2) \, \phi_1(\vec{r}_1) \, \phi_2(\vec{r}_2)$$

$\langle 21 | v | 12 \rangle$

Exchange Term.

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

$$= \langle pq | v | pq \rangle - \langle qp | v | pq \rangle$$

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

for N Body Slater Determinants

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

for 6 particle there will be 6×6 element so we want to compactify this problem into a

Small Space:

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

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

$\hat{A}$ = Antisymmetrization property (operator)

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

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