Fock space

$$\mathcal{U}_d = \text{span}\{\phi_1(\vec{x}), \cdots, \phi_d(\vec{x})\}.$$

$$\mathcal{A}_{N,d} = \bigwedge^N \mathcal{U}_d$$

$$\mathcal{F}_{\mathcal{U}} = \bigoplus_M^d \mathcal{A}_{M,d} = \{|\Psi\rangle = |\Psi_0\rangle \oplus \cdots \oplus |\Psi_d\rangle \mid \Psi_M \in \mathcal{A}_{M,d}\}.$$

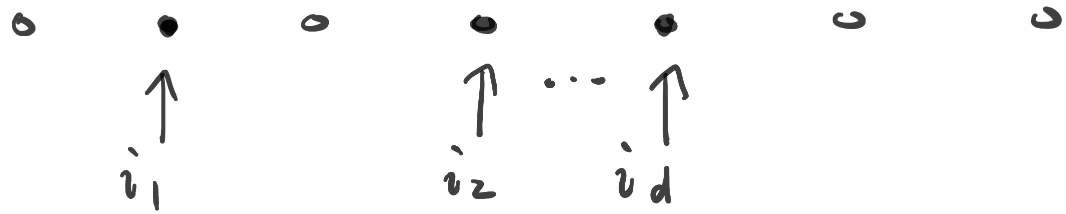
$$\dim \mathcal{F}_d = 2^d \gg \binom{d}{N}.$$

Inner product, $\Psi, \Phi \in \mathcal{F}_d$.

$$\langle \Phi | \Psi \rangle = \sum_{M=0}^{d} \langle \Phi_M | \Psi_M \rangle$$

$$\langle \Psi | \Psi \rangle = 0 \Rightarrow \langle \Psi_M | \Psi_M \rangle = 0. \ \forall M.$$

Slater $\Phi_{[i_1,\cdots,i_N]} =: |n_1 \cdots n_d\rangle$, $n_i \in \{0,1\}$.



$$\mathcal{F}_{\cup} = \Big\{ |\Psi\rangle \;\Big|\; |\Psi\rangle = \sum_{n_1,\cdots,n_d} \Psi(n_1,\cdots,n_d)\, |n_1,\cdots n_d\rangle$$

$$\Psi(n_1,\cdots,n_d) \in \mathbb{C} \Big\}$$

$$\cong \mathbb{C}^{2^d} \cong \bigotimes^{d} \mathbb{C}^2$$

$|0\rangle \sim \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $|1\rangle \sim \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $\Psi \in \bigotimes^{d} \mathbb{C}^2$.

$$\langle \Phi | \Psi \rangle = \sum_{n_1, \dots, n_d} \Phi^*(n_1, \dots, n_d)\, \Psi(n_1, \dots, n_d)$$

Operator. bake in anti-symmetry.

annihilation

$$c_k | n_1 \cdots n_k \cdots n_d \rangle = \begin{cases} (-1)^{P_k} | n_1 \cdots n_{k-1}, 0, n_{k+1}, \dots, n_d \rangle, & n_k = 0 \\ 0, & n_k = 1 \end{cases}$$

$P_k = \sum_{i=1}^{k-1} n_i$: parity. $A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$

$$c_k = \sigma_z \otimes \cdots \otimes \sigma_z \otimes \underset{\underset{k}{\uparrow}}{A} \otimes I \otimes \cdots \otimes I = \sigma_z^{k-1} \otimes A \otimes I^{d-k}$$

creation.

$$c_k^{\dagger} |n_1 \cdots n_k \cdots n_d\rangle = \begin{cases} (-1)^{P_k} |n_1 \cdots n_{k-1}, 1, n_{k+1}, \cdots, n_d\rangle, & n_k = 0 \\ 1 & , n_k = 1 \end{cases}$$

$$A^* = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$c_k^{\dagger} = \sigma_z \otimes \cdots \otimes \sigma_z \otimes \underset{\underset{k.}{\uparrow}}{A^*} \otimes I \otimes \cdots \otimes I = \sigma_z^{k-1} \otimes A^* \otimes I^{d-k}$$

<u>Thm</u>. $\{c_i^{\dagger}, c_j\} = \delta_{ij}$, $\{c_i, c_j\} = \{c_i^{\dagger}, c_j^{\dagger}\} = 0$.

Pf: ① $i < j$

$$c_i^\dagger c_j + c_j c_i^\dagger = I^{i-1} \otimes (A^* \sigma_z) \otimes \sigma_z^{j-i} \otimes A \otimes I^{d-j}$$

$$+ I^{i-1} \otimes (\sigma_z A^*) \otimes \sigma_z^{j-i} \otimes A \otimes I^{d-j}$$

$$= I^{i-1} \otimes \{A^*, \sigma_z\} \otimes \sigma_z^{j-i} \otimes A \otimes I^{d-j} = 0.$$

$$\{A^*, \sigma_z\} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$= 0$. similar $\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$.

② $i=j$.

$$c_i^\dagger c_i + c_i c_i^\dagger = I^{i-1} \otimes \{A^*, A\} \otimes I^{d-i} = I^d =: \mathbb{1}.$$

$$\{A^*, A\} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} = I. \quad \ldots$$

$$\{c_i, c_i\} = \{c_i^\dagger, c_i^\dagger\} = 0. \qquad \square.$$

Thm. $c_k^\dagger c_k | n_1 \cdots n_k \cdots n_d \rangle = n_k | n_1 \cdots n_d \rangle$

Pf: $\hat{n} = A^* A = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$, $\hat{n} | n \rangle = n | n \rangle$

$$c_k^\dagger c_k = I^{k-1} \otimes \hat{n} \otimes I^{d-k} := \hat{n}_k \qquad \square.$$

Thm. $| n_1 \cdots n_d \rangle = (c_1^\dagger)^{n_1} \cdots (c_d^\dagger)^{n_d} | 0 \rangle$

note order $\longrightarrow$ parity.

One body $\quad O(x) \longrightarrow O_M = \sum_{k=1}^{M} O(\vec{x}_k)$

$$O_{ij} = \langle \phi_i | O | \phi_j \rangle = \int d\vec{x} \; \phi_i^*(\vec{x}) \, O(\vec{x}) \, \phi_j(\vec{x})$$

$|n_1 \cdots n_d\rangle \quad , \quad \sum n_k = M . \qquad i_1, \cdots, i_M .$

$$(O \phi_j)(\vec{x}) \longrightarrow \sum_i \phi_i(\vec{x}) \langle \phi_i | O | \phi_j \rangle = \sum_i \phi_i(\vec{x}) O_{ij} .$$

$$(O_M \Phi_{[i_1 \cdots i_M]})(\vec{x}_1, \cdots, \vec{x}_M) = \sum_{k=1}^{M} O(\vec{x}_k) \, \Phi_{[i_1, \cdots, i_M]}(\vec{x}_1, \cdots, \vec{x}_M)$$

$$\longrightarrow \sum_{k=1}^{M} \sum_i \Phi_{[i_1, \cdots, i_{k-1}, i, i_{k+1}, \cdots, i_M]}(\vec{x}_1, \cdots, \vec{x}_M) \, O_{i i_k}$$

or $\hat{O}\, c_{i_1}^\dagger \cdots c_{i_M}^\dagger |0\rangle = \sum_{k=1}^{M} \sum_{i} O_{i i_k}\, c_{i_1}^\dagger \cdots c_{i_{k-1}}^\dagger c_i^\dagger c_{i_{k+1}}^\dagger \cdots c_{i_M}^\dagger |0\rangle$.

__Lem__. $[c_i^\dagger c_j, c_k^\dagger] = c_i^\dagger \delta_{jk}$.

Pf: $c_i^\dagger c_j c_k^\dagger - c_k^\dagger c_i^\dagger c_j$

$= -c_i^\dagger c_k^\dagger c_j + c_i^\dagger \delta_{jk} - c_k^\dagger c_i^\dagger c_j = c_i^\dagger \delta_{jk}$.

Thm. $\hat{O} = \sum_{ij} c_i^\dagger c_j \, O_{ij}$

Pf: $\hat{O} \, c_{i_1}^\dagger \cdots c_{i_M}^\dagger |0\rangle$

$$= [\hat{O}, c_{i_1}^\dagger] \, c_{i_2}^\dagger \cdots c_{i_M}^\dagger |0\rangle$$

$$+ \, c_{i_1}^\dagger \, \hat{O} \, c_{i_2}^\dagger \cdots c_{i_M}^\dagger |0\rangle$$

$$= \sum_i c_i^\dagger c_{i_2}^\dagger \cdots c_{i_M}^\dagger |0\rangle \, O_{i i_1} + c_{i_1}^\dagger [\hat{O}, c_{i_2}^\dagger] \, c_{i_3}^\dagger \cdots c_{i_M}^\dagger |0\rangle$$

$$+ \, c_{i_1}^\dagger c_{i_2}^\dagger \, \hat{O} \, c_{i_3}^\dagger \cdots c_{i_M}^\dagger |0\rangle$$

$$= \sum_{K=1}^{M} \sum_i O_{i i_K} \, c_{i_1}^\dagger \cdots c_i^\dagger \cdots c_{i_M}^\dagger |0\rangle + c_{i_1}^\dagger \cdots \cancel{c_{i_M}^\dagger \hat{O}} |0\rangle$$

$\square$

Ex. $H_{0,N} = \sum_{k=1}^{N} \left(-\frac{1}{2}\Delta_{\vec{r}_k} + V_{ext}(\vec{r}_k) \right)$

$$H_{0,N} = \sum_{ij} h_{ij} \, c_i^{\dagger} c_j$$

$$h_{ij} = \int d\vec{x} \; \phi_i^{*}(\vec{x}) \left(-\frac{1}{2}\Delta_{\vec{r}} + V_{ext}(\vec{r}) \right) \phi_j(\vec{x})$$

Two-body.

$$O_M = \sum_{1 \le k < l \le M} O(\vec{x}_k, \vec{x}_l).$$

$$O_{pqrs} = \int d\vec{x}\, d\vec{x}'\, \varphi_p^*(\vec{x})\, \varphi_q^*(\vec{x}')\, O(\vec{x}, \vec{x}')\, \varphi_r(\vec{x})\, \varphi_s(\vec{x}')$$

$$\left(O_M \Phi_{[i_1 \cdots i_M]}\right)(\vec{x}_1, \cdots, \vec{x}_M)$$

$$= \sum_{1 \le k < l \le M} \sum_{pq} \Phi_{[i_1, \cdots, \underset{\substack{\uparrow \\ k}}{p}, \cdots, \underset{\substack{\uparrow \\ l}}{q}, \cdots, i_M]}(\vec{x}_1, \cdots, \vec{x}_M)\, O_{pq i_k i_l}$$

(exer)

$$\hat{O}\, c_{i_1}^\dagger \cdots c_{i_M}^\dagger |0\rangle = \sum_{1 \le k < l \le M} \sum_{pq} O_{pq i_k i_l}\, c_{i_1}^\dagger \cdots c_p^\dagger \cdots c_q^\dagger \cdots c_{i_M}^\dagger |0\rangle$$

Thm. $\hat{O} = \frac{1}{2} \sum_{pqrs} c_p^\dagger c_q^\dagger c_s c_r \; O_{pqrs}$.

Pf: First show

$$[c_p^\dagger c_q^\dagger c_s c_r, c_k^\dagger] = c_p^\dagger c_q^\dagger c_s \delta_{kr} - c_p^\dagger c_q^\dagger c_r \delta_{sr}$$

$$\Rightarrow [\hat{O}, c_k^\dagger] = \frac{1}{2}\sum_{pqs} c_p^\dagger c_q^\dagger c_s \left(O_{pqks} - O_{pqsk}\right)$$

exchang p, q

$O_{pqrs} = O_{qpsr}$

$$= \sum_{pqs} c_p^\dagger c_q^\dagger c_s \; O_{pqks}$$

$$\hat{O}\, c_{i_1}^\dagger \cdots c_{i_M}^\dagger |0\rangle$$

$$= \sum_{pqs} c_p^\dagger \left(c_q^\dagger c_s\right) c_{i_2}^\dagger \cdots c_{i_M}^\dagger |0\rangle \, O_{pqi_1s}$$

single particle.

$$+ \; c_{i_1}^\dagger \, \hat{O} \, c_{i_2}^\dagger \cdots c_{i_M}^\dagger |0\rangle$$

$$= \sum_{pq} \sum_{l=2}^{M} c_p^\dagger \, c_{i_2}^\dagger \cdots c_q^\dagger \cdots c_{i_M}^\dagger |0\rangle \; O_{pqi_1i_l}$$

$$+ \; c_{i_1}^\dagger \, \hat{O} \, c_{i_2}^\dagger \cdots c_{i_M}^\dagger |0\rangle$$

induction

$$= \sum_{pq} \sum_{1 \leq k < l \leq M} c_{i_1}^\dagger \cdots c_p^\dagger \cdots c_q^\dagger \cdots c_{i_M}^\dagger \quad O_{pqi_ki_l} \qquad \square$$

$$H_N = \sum_{i=1}^{N} \left(-\frac{1}{2}\Delta_{\vec{r}_i} + V_{ext}(\vec{r}_i)\right) + \sum_{1 \leq i < j \leq N} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

$$\longrightarrow H = \sum_{pq} h_{pq} c_p^\dagger c_q + \frac{1}{2}\sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_s c_r .$$

$$h_{pq} = \int \phi_i^*(\vec{x}) \left(-\frac{1}{2}\Delta_{\vec{r}} + V_{ext}(\vec{r})\right) \phi_j(\vec{x})\, d\vec{x}$$

$$V_{pqrs} = \int \phi_p^*(\vec{x})\, \phi_q^*(\vec{x}')\, \frac{1}{|\vec{x} - \vec{x}'|}\, \phi_r(\vec{x})\, \phi_s(\vec{x}')\, d\vec{x}\, d\vec{x}'.$$