

Fock space

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

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

$$\mathcal{F}_d = \bigoplus_m^d \mathcal{A}_{m,d} = \{ |\underline{\Psi}\rangle = |\underline{\Psi}_0\rangle \oplus \dots \oplus |\underline{\Psi}_d\rangle \mid \underline{\Psi}_m \in \mathcal{A}_{m,d} \}.$$

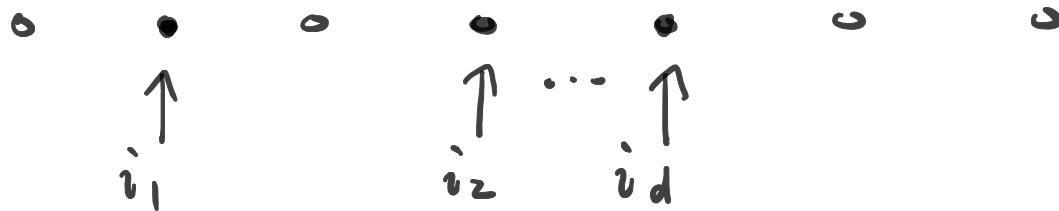
$$\dim \mathcal{F}_d = 2^d \gg \binom{d}{N}.$$

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

$$\langle \underline{\Phi} | \underline{\Psi} \rangle = \sum_{M=0}^d \langle \underline{\Phi}_M | \underline{\Psi}_M \rangle$$

$$\langle \underline{\Psi} | \underline{\Psi} \rangle = 0 \Rightarrow \langle \underline{\Psi}_M | \underline{\Psi}_M \rangle = 0 \quad \forall M.$$

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



$$\mathcal{F}_\perp = \{ |\Psi\rangle \mid |\Psi\rangle = \sum_{n_1, \dots, n_d} \Psi(n_1, \dots, n_d) |n_1, \dots, n_d\rangle$$

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

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

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

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

Operator. take in anti-symmetry.

annihilation

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

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

$$C_k = \sigma_z \otimes \dots \otimes \sigma_z \otimes \underset{\substack{\uparrow \\ k}}{A} \otimes I \otimes \dots \otimes I = \sigma_z^{k-1} \otimes A \otimes I^{d-k}$$

creation.

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

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

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

Thm. $\{c_i^\dagger, c_j\} = \delta_{ij}$, $\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$.

Pf: ^① $i < j$

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

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

$$\{A^*, \sigma_z\} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \\ = 0. \quad \text{similar } \{C_i, C_j\} = \{C_i^\dagger, C_j^\dagger\} = 0.$$

② $i=j$.

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

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

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

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

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

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

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

↑
note order \rightarrow parity.

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

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

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

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

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

$$\rightarrow \sum_{k=1}^M \sum_i \bar{\Phi}_{[i_1, \dots, i_{k-1}, i, i_{k+1}, \dots, i_M]}(\vec{x}_1, \dots, \vec{x}_M) O_{ii_k}$$

$$\hat{O} c_{i_1}^+ \cdots c_{i_M}^+ |0\rangle = \sum_{k=1}^M \sum_i O_{ii_k} c_{i_1}^+ \cdots c_{i_{k-1}}^+ c_i^+ c_{i_{k+1}}^+ \cdots c_{i_M}^+ |0\rangle.$$

Lem. $[c_i^+ c_j, c_k^+] = c_i^+ \delta_{jk}.$

Pf: $c_i^+ c_j c_k^+ - c_k^+ c_i^+ c_j$

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

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

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

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

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

$$= \sum_i c_i^\dagger c_{i_2}^\dagger \cdots c_{i_m}^\dagger |0\rangle O_{ii_1} + c_{i_1}^\dagger [\hat{O}, c_{i_2}^\dagger] c_{i_3}^\dagger \cdots c_{i_m}^\dagger |0\rangle$$

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

$$= \sum_{K=1}^M \sum_i O_{ii_K} c_i^\dagger \cdots c_{i_1}^\dagger \cdots c_{i_m}^\dagger |0\rangle + c_{i_1}^\dagger \cdots \cancel{c_{i_m}^\dagger \hat{O}} |0\rangle \quad \square$$

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

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

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

Two-body.

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

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

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

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

(exer)

$$\hat{O} c_{i_1}^\dagger \cdots c_{i_m}^\dagger |0\rangle = \sum_{1 \leq k \leq LSM} \sum_{pq} O_{pq i_k i_k} c_{i_1}^\dagger \cdots c_p^\dagger \cdots c_q^\dagger \cdots c_{i_m}^\dagger |0\rangle$$

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

Pf: First show

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

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

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

exchange p, q

$$O_{pqrs} = O_{qp sr}$$

$$\hat{O} c_{i_1}^\dagger \dots c_{i_m}^\dagger |0\rangle$$

$$= \sum_{pqs} c_p^\dagger (c_q^\dagger c_s) c_{i_2}^\dagger \dots c_{i_m}^\dagger |0\rangle O_{pq i_1 s}$$

single particle.

$$+ c_{i_1}^\dagger \hat{O} c_{i_2}^\dagger \dots c_{i_m}^\dagger |0\rangle$$

$$= \sum_{pq} \sum_{l=2}^m c_p^\dagger c_{i_2}^\dagger \dots c_q^\dagger \dots c_{i_m}^\dagger |0\rangle O_{pq i_1 i_l}$$

$$+ c_{i_1}^\dagger \hat{O} c_{i_2}^\dagger \dots c_{i_m}^\dagger |0\rangle$$

$$\stackrel{\text{induction}}{=} \sum_{pq} \sum_{1 \leq k < l \leq M} c_{i_1}^+ \cdots c_p^+ \cdots c_q^+ \cdots c_{i_n}^+ \quad O_{pq i_k i_l} \quad \square$$

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

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

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

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