

• Two-body operators and creation/annihilation operators:

First Pair number operator $\{|\alpha\rangle, |\beta\rangle\}$ $|\alpha_1 \dots \alpha_N\rangle$

$$\left. \begin{array}{l} \text{if } |\alpha\rangle \neq |\beta\rangle \\ \text{if } |\alpha\rangle = |\beta\rangle \end{array} \right\} \begin{array}{l} n_\alpha n_\beta \\ n_\alpha (n_\alpha - 1) \end{array}$$

$$\hat{P}_{\alpha\beta} = \hat{n}_\alpha \hat{n}_\beta - \delta_{\alpha\beta} \hat{n}_\beta$$

Some rewriting: $\hat{P}_{\alpha\beta} = a_\alpha^\dagger (a_\alpha a_\beta^\dagger) a_\beta - \delta_{\alpha\beta} a_\alpha^\dagger a_\alpha = a_\alpha^\dagger (\sum_{\alpha\beta} a_\alpha^\dagger a_\alpha + \delta_{\alpha\beta}) a_\beta - \delta_{\alpha\beta} a_\alpha^\dagger a_\alpha$

$$= \sum_{\alpha\beta} a_\alpha^\dagger a_\beta^\dagger \underbrace{a_\alpha a_\beta}_{\sum_{\alpha\beta} a_\alpha a_\beta} = a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha$$

Now: take an arbitrary 2-body op, $\hat{V} = \frac{1}{2} \sum_{i \neq j} \hat{V}_{ij}$ and the corresponding eigenbasis.

$$\left. \begin{array}{l} \hat{V} |\alpha\beta\rangle = V_{\alpha\beta} |\alpha\beta\rangle \\ V_{\alpha\beta} = \langle \alpha\beta | \hat{V} | \alpha\beta \rangle \end{array} \right\}$$

$$\begin{aligned} \hat{V} |\alpha_1 \dots \alpha_N\rangle &= \hat{V} \sum_{\mathcal{P}} \frac{1}{\sqrt{N!}} \mathcal{P} |\alpha_{\mathcal{P}1} \dots \alpha_{\mathcal{P}N}\rangle = \frac{1}{2} \sum_{i \neq j} \hat{V}_{ij} \sum_{\mathcal{P}} \frac{1}{\sqrt{N!}} \mathcal{P} |\alpha_{\mathcal{P}1} \dots \alpha_{\mathcal{P}N}\rangle = \\ &= \sum_{\mathcal{P}} \frac{1}{\sqrt{N!}} \mathcal{P} \left[\frac{1}{2} \sum_{i \neq j} V_{\alpha_{\mathcal{P}i} \alpha_{\mathcal{P}j}} |\alpha_{\mathcal{P}1} \dots \alpha_{\mathcal{P}N}\rangle \right] = \\ &= \frac{1}{2} \sum_{i \neq j} V_{\alpha_i \alpha_j} = \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta} \hat{P}_{\alpha\beta} \end{aligned}$$

$$\hat{V} |\alpha_1 \dots \alpha_N\rangle = \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta} \underbrace{\hat{P}_{\alpha\beta} |\alpha_1 \dots \alpha_N\rangle}_{\hat{P}_{\alpha\beta} |\alpha_1 \dots \alpha_N\rangle} = \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta} \hat{P}_{\alpha\beta} |\alpha_1 \dots \alpha_N\rangle$$

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta} \hat{P}_{\alpha\beta} = \frac{1}{2} \sum_{\alpha\beta} (\alpha\beta | \hat{V} | \alpha\beta) a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha$$

arbitrary basis

(2)

$$a_{\alpha}^{\dagger} = \sum_{\tilde{\alpha}} \langle \tilde{\alpha} | \alpha \rangle a_{\tilde{\alpha}}^{\dagger}$$

$$a_{\alpha} = \sum_{\tilde{\alpha}} \langle \alpha | \tilde{\alpha} \rangle a_{\tilde{\alpha}}$$

$$\hat{V} = \frac{1}{2} \sum_{\alpha \beta} V_{\alpha \beta} \sum_{\tilde{\alpha}_1} \sum_{\tilde{\alpha}_2} \sum_{\tilde{\beta}_1} \sum_{\tilde{\beta}_2} \langle \tilde{\alpha}_1 | \alpha \rangle a_{\tilde{\alpha}_1}^{\dagger} \langle \tilde{\beta}_1 | \beta \rangle a_{\tilde{\beta}_1}^{\dagger} \langle \tilde{\beta}_2 | \beta \rangle a_{\tilde{\beta}_2} \langle \alpha | \tilde{\alpha}_2 \rangle a_{\tilde{\alpha}_2} =$$

$$= \frac{1}{2} \sum_{\tilde{\alpha}_1 \tilde{\alpha}_2} \sum_{\tilde{\beta}_1 \tilde{\beta}_2} \left(\langle \tilde{\alpha}_1 | \otimes \langle \tilde{\beta}_1 | \right) \left[\sum_{\alpha \beta} V_{\alpha \beta} | \alpha \rangle \otimes | \beta \rangle \langle \alpha | \otimes \langle \beta | \right] \left(| \tilde{\alpha}_2 \rangle \otimes | \tilde{\beta}_2 \rangle \right) \cdot$$

$\cdot a_{\tilde{\alpha}_1}^{\dagger} a_{\tilde{\beta}_1}^{\dagger} a_{\tilde{\beta}_2} a_{\tilde{\alpha}_2}$

$$\hat{V} = \frac{1}{2} \sum_{\tilde{\alpha}_1 \tilde{\alpha}_2 \tilde{\beta}_1 \tilde{\beta}_2} \left(\tilde{\alpha}_1 \tilde{\beta}_1 | \hat{V} | \tilde{\alpha}_2 \tilde{\beta}_2 \right) a_{\tilde{\alpha}_1}^{\dagger} a_{\tilde{\beta}_1}^{\dagger} a_{\tilde{\beta}_2} a_{\tilde{\alpha}_2}$$

$$\hat{V} = \frac{1}{2} \sum_{\beta_1 \beta_2 \beta_3 \beta_4} \left(\beta_1 \beta_2 | \hat{V} | \beta_4 \beta_3 \right) a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} a_{\beta_3} a_{\beta_4}$$

Important example

2-body interaction operator (such as Coulomb)

\hat{V} - diagonal in position basis $|\bar{r}, \sigma\rangle$

$$\langle \bar{r}_1 \sigma_1 \bar{r}_2 \sigma_2 | \hat{V} | \bar{r}_3 \sigma_3 \bar{r}_4 \sigma_4 \rangle = \underbrace{V(\bar{r}_3 - \bar{r}_4)}_{\text{for Coulomb}} \delta(\bar{r}_1 - \bar{r}_3) \delta(\bar{r}_2 - \bar{r}_4) \delta_{\sigma_1 \sigma_3} \delta_{\sigma_2 \sigma_4}$$

this is $\frac{e^2}{|\bar{r}_3 - \bar{r}_4|} = \frac{e^2}{4\pi\epsilon_0 |\bar{r}_3 - \bar{r}_4|}$

$$\hat{V} = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d\bar{r}_1 \int d\bar{r}_2 V(\bar{r}_1 - \bar{r}_2) \bar{\Psi}_{\sigma_1}^{\dagger}(\bar{r}_1) \bar{\Psi}_{\sigma_2}^{\dagger}(\bar{r}_2) \bar{\Psi}_{\sigma_2}(\bar{r}_2) \bar{\Psi}_{\sigma_1}(\bar{r}_1)$$

\hat{V} in position basis.

Transformation to momentum basis

3

$$\hat{V} = \frac{1}{2} \sum_{\vec{k}_3 \sigma_3} \sum_{\vec{k}_2 \sigma_2} \sum_{\vec{k}_3 \sigma_3} \sum_{\vec{k}_4 \sigma_4} (\bar{k}_3 \sigma_3 \bar{k}_4 \sigma_4 | \hat{V} | \bar{k}_1 \sigma_1 \bar{k}_2 \sigma_2) a_{\vec{k}_3 \sigma_3}^\dagger a_{\vec{k}_4 \sigma_4}^\dagger a_{\vec{k}_2 \sigma_2} a_{\vec{k}_1 \sigma_1}$$

↓

$$\left. \begin{aligned} & \sum_{\vec{q} \sigma_2'} \int d\vec{r}_1 \int d\vec{r}_2 | \vec{r}_1 \sigma_1' \vec{r}_2 \sigma_2' \rangle V(\vec{r}_1 - \vec{r}_2) \langle \vec{r}_1 \sigma_1' \vec{r}_2 \sigma_2' | \\ & \langle \vec{k}_i | \vec{r}_i \rangle = \frac{1}{\sqrt{V}} e^{-i\vec{k}_i \cdot \vec{r}_i} \end{aligned} \right\}$$

$$= \frac{1}{2} \frac{1}{V^2} \sum_{\sigma_1 \sigma_2} \sum_{\vec{k}_1 \vec{k}_2 \vec{k}_3 \vec{k}_4} \int d\vec{r}_1 \int d\vec{r}_2 V(\vec{r}_1 - \vec{r}_2) e^{i(-\vec{r}_1 \vec{k}_3 - \vec{r}_2 \vec{k}_4 + \vec{r}_1 \vec{k}_1 + \vec{r}_2 \vec{k}_2)} a_{\vec{k}_3 \sigma_1}^\dagger a_{\vec{k}_4 \sigma_2}^\dagger a_{\vec{k}_2 \sigma_2} a_{\vec{k}_1 \sigma_1} =$$

$$\left. \begin{aligned} \vec{r} &:= \vec{r}_2 - \vec{r}_1 & e^{i(\dots)} &= e^{i(\vec{r}_2 - \vec{r}_1)(\vec{k}_2 - \vec{k}_4)} e^{i(\vec{k}_1 \vec{r}_1 - \vec{k}_3 \vec{r}_1 + \vec{k}_2 \vec{r}_1 - \vec{k}_4 \vec{r}_1)} = \\ \vec{q} &:= \vec{k}_2 - \vec{k}_4 & &= e^{i(\vec{k}_2 - \vec{k}_4)(\vec{r}_2 - \vec{r}_1)} e^{i(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4) \vec{r}_1} \end{aligned} \right\}$$

$$\int d\vec{r}_1 \int d\vec{r}_2 \rightarrow \int d\vec{r} \int d\vec{r}_1$$

- $\int d\vec{r} V(\vec{r}) e^{i\vec{q} \cdot \vec{r}} =: V_{\vec{q}}$
- $\int d\vec{r}_1 e^{i(\vec{k}_1 - \vec{k}_3 + \vec{q}) \cdot \vec{r}_1} = V \delta_{\vec{k}_1 - \vec{k}_3 + \vec{q}, 0}$

$$= \frac{1}{2V} \sum_{\sigma_1 \sigma_2} \sum_{\vec{k}_1 \dots \vec{k}_4} \delta_{\vec{k}_1 - \vec{k}_3 + \vec{q}, 0} V_{\vec{q}} a_{\vec{k}_3 \sigma_1}^\dagger a_{\vec{k}_4 \sigma_2}^\dagger a_{\vec{k}_2 \sigma_2} a_{\vec{k}_1 \sigma_1} = \left. \begin{aligned} & \vec{k}_q = \vec{k}_2 - \vec{q} \\ & \vec{k}_3 = \vec{k}_1 + \vec{q} \text{ (from } \delta \dots \text{)} \\ & \sum_{\vec{k}_4} \rightarrow \sum_{\vec{q}} \end{aligned} \right\} =$$

$$= \frac{1}{2V} \sum_{\sigma_1 \sigma_2} \sum_{\vec{k}_1 \vec{k}_2 \vec{q}} V_{\vec{q}} a_{\vec{k}_1 + \vec{q} \sigma_1}^\dagger a_{\vec{k}_2 - \vec{q} \sigma_2}^\dagger a_{\vec{k}_2 \sigma_2} a_{\vec{k}_1 \sigma_1}$$

