4.3 Single- and many-particle operators

- example: $$H = \sum_{\alpha=1}^{N} \left(\underset{\substack{\uparrow}}{\frac{\vec{p}_\alpha^{\,2}}{2m}} + \underset{\substack{\uparrow}}{U(\vec{x}_\alpha)} \right) + \frac{1}{2} \sum_{\alpha \neq \beta} \underset{\substack{\uparrow}}{V(\vec{x}_\alpha, \vec{x}_\beta)}$$

  one-particle operators   two-particle operator

goal: express H in terms of creation and annihilation operators

1. single-particle operators: $\hat{T} = \sum_\alpha \hat{t}_\alpha$ (e.g., $\hat{t}_\alpha = \frac{\vec{p}_\alpha^{\,2}}{2m}$)

- Consider a single-particle system first ($N = 1$) ➞ $\hat{t}_\alpha = \hat{t}_1 \equiv \hat{t}$

  Let $t_{ij} \equiv \langle i|\hat{t}|j\rangle$

  Then: $$\hat{t} = \Big(\sum_i |i\rangle\langle i| \Big)\, \hat{t}\, \Big(\sum_j |j\rangle\langle j| \Big) = \sum_{ij} |i\rangle\, t_{ij}\, \langle j| = \sum_{ij} t_{ij}\, |i\rangle\langle j|$$

  $$\Rightarrow \langle i|\hat{t}|j\rangle = \sum_{i'j'} t_{i'j'}\, \underbrace{\langle i|i'\rangle}_{\delta_{ii'}}\, \underbrace{\langle j'|j\rangle}_{\delta_{j'j}} = t_{ij} \quad \checkmark$$

single-particle system: $\hat{t} = \sum_{ij} t_{ij} \, |i\rangle\langle j|$

→ *N*-particle system: $\hat{T} = \sum_{\alpha=1}^{N} \hat{t}_\alpha = \sum_{ij} t_{ij} \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha$

- $\sum_\alpha |i\rangle_\alpha \langle j|_\alpha$ symmetric under permutations of the particles

  $$\Rightarrow \quad \left[P, \sum_\alpha |i\rangle_\alpha \langle j|_\alpha\right] = 0 \Rightarrow \quad \left[S_\pm, \sum_\alpha |i\rangle_\alpha \langle j|_\alpha\right] = 0$$

- bosons:

$$\sum_\alpha |i\rangle_\alpha \langle j|_\alpha \, |n_1, n_2, \dots\rangle = \sum_\alpha |i\rangle_\alpha \langle j|_\alpha \, \frac{1}{\sqrt{n_1! n_2! \dots}} \, S_+ |i_1, \dots, i_N\rangle$$

$$= \frac{1}{\sqrt{n_1! n_2! \dots}} \, S_+ \sum_\alpha |i\rangle_\alpha \langle j|_\alpha \, |i_1, \dots, i_N\rangle$$

(with a suitable *N*-particle state $|i_1, \dots, i_N\rangle$)

$$\Rightarrow \sum_\alpha |i\rangle_\alpha \langle j|_\alpha \, |n_1, n_2, \ldots\rangle = \frac{1}{\sqrt{n_1! n_2! \ldots}} S_+ \sum_\alpha |i\rangle_\alpha \langle j|_\alpha \, |i_1\rangle_1 \ldots |i_N\rangle_N$$

(i) <u>$i \neq j$:</u>

$$= \underbrace{\sqrt{n_i+1}\,\frac{1}{\sqrt{n_j}}}_{\text{correct normalization of the new state}} \quad \underbrace{n_j\,|\ldots, n_i+1, \ldots, n_j-1, \ldots\rangle}_{\text{In } n_j \text{ terms } |j\rangle \text{ gets replaced by } |i\rangle}$$

$$= \sqrt{n_i+1}\sqrt{n_j}\,|\ldots, n_i+1, \ldots, n_j-1, \ldots\rangle$$

$$= a_i^\dagger \, a_j \, |\ldots, n_i, \ldots, n_j, \ldots\rangle$$

(ii) <u>$i = j$:</u>

$$= \underbrace{n_i\,|\ldots, n_i, \ldots\rangle}_{\text{In } n_i \text{ terms } |i\rangle \text{ gets ``replaced'' by } |i\rangle.} \qquad = a_i^\dagger \, a_i \, |\ldots, n_i, \ldots\rangle$$

$$\Rightarrow \sum_\alpha |i\rangle_\alpha \langle j|_\alpha = a_i^\dagger \, a_j \quad \text{for all } i, j.$$

This also holds for fermions (→ exercises).

- We had: $\hat{T} = \sum_{ij} t_{ij} \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha , \qquad \sum_\alpha |i\rangle_\alpha \langle j|_\alpha = a_i^\dagger\, a_j$

$$\Rightarrow \quad \boxed{\hat{T} = \sum_{ij} t_{ij}\, a_i^\dagger\, a_j \equiv \sum_{ij} \langle i|\hat{t}|j\rangle\, a_i^\dagger\, a_j}$$

- special case: $t_{ij} = \varepsilon_i \delta_{ij}$

  (i.e., the single-particle operator is diagonal in the single-particle basis)

  $$\Rightarrow \quad \hat{T} = \sum_i \varepsilon_i\, a_i^\dagger\, a_i = \sum_i \varepsilon_i\, \hat{n}_i$$

  The total energy of particles which do not interact with each other is the sum of the single-particle energies. ✓

2. Two-particle operators: $\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} \hat{f}_{\alpha\beta}$ (e.g., $\hat{f}_{\alpha\beta} = V(\vec{x}_\alpha, \vec{x}_\beta)$)

- Analogously to the single-particle operators we write:

$$\hat{F} = \frac{1}{2} \sum_{ijmn} \langle i, j | \hat{f} | m, n \rangle \sum_{\alpha \neq \beta} |i\rangle_\alpha |j\rangle_\beta \langle m|_\alpha \langle n|_\beta$$

  - Meaning of the two-particle matrix elements $\langle i, j | \hat{f} | m, n \rangle$: see later

- $\sum_{\alpha \neq \beta} |i\rangle_\alpha |j\rangle_\beta \langle m|_\alpha \langle n|_\beta = \sum_{\alpha \neq \beta} |i\rangle_\alpha \langle m|_\alpha \; |j\rangle_\beta \langle n|_\beta$

$$= \sum_{\alpha,\beta} |i\rangle_\alpha \langle m|_\alpha \; |j\rangle_\beta \langle n|_\beta - \sum_{\alpha} |i\rangle_\alpha \langle m|_\alpha \; |j\rangle_\alpha \langle n|_\alpha$$

$$= \sum_{\alpha} |i\rangle_\alpha \langle m|_\alpha \sum_{\beta} |j\rangle_\beta \langle n|_\beta - \sum_{\alpha} |i\rangle_\alpha \underbrace{\langle m|j\rangle}_{\delta_{mj}} \langle n|_\alpha$$

$$= a_i^\dagger a_m \, a_j^\dagger a_n - a_i^\dagger \delta_{mj} \, a_n$$

$$\sum_{\alpha \neq \beta} |i\rangle_\alpha |j\rangle_\beta \langle m|_\alpha \langle n|_\beta = a_i^\dagger a_m \, a_j^\dagger a_n - a_i^\dagger \delta_{mj} \, a_n$$

$$\delta_{mj} = \begin{cases} \left[a_m, a_j^\dagger\right] & \text{for bosons} \\ \left\{a_m, a_j^\dagger\right\} & \text{for fermions} \end{cases}$$

$$\Rightarrow \sum_{\alpha \neq \beta} |i\rangle_\alpha |j\rangle_\beta \langle m|_\alpha \langle n|_\beta = \pm a_i^\dagger a_j^\dagger a_m a_n = a_i^\dagger a_j^\dagger a_n a_m$$

- $\hat{F} = \frac{1}{2} \sum_{ijmn} \langle i, j | \hat{f} | m, n \rangle \sum_{\alpha \neq \beta} |i\rangle_\alpha |j\rangle_\beta \langle m|_\alpha \langle n|_\beta$

$$\Rightarrow \quad \boxed{\hat{F} = \frac{1}{2} \sum_{ijmn} \langle i, j | \hat{f} | m, n \rangle \, a_i^\dagger a_j^\dagger a_n a_m}$$

Two-particle matrix elements

- example: $\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} \hat{V}(\hat{\vec{x}}_\alpha, \hat{\vec{x}}_\beta) = \frac{1}{2} \sum_{\alpha \neq \beta} \frac{e^2}{|\hat{\vec{x}}_\alpha - \hat{\vec{x}}_\beta|}$, $\quad \hat{\vec{x}}_\lambda$: position op. for particle λ

$$= \frac{1}{2} \sum_{\alpha \neq \beta} \hat{f}_{\alpha\beta} \quad \Rightarrow \quad \hat{f}_{\alpha\beta} = \hat{V}(\hat{\vec{x}}_\alpha, \hat{\vec{x}}_\beta)$$

- two-particle matrix elements in position space:

$$\begin{aligned} \langle \vec{x}_1, \vec{x}_2 | \hat{V}(\underset{\substack{\uparrow \\ \text{1st particle}}}{\hat{\vec{x}}_{(1)}}, \underset{\substack{\uparrow \\ \text{2nd particle}}}{\hat{\vec{x}}_{(2)}}) | \vec{x}_3, \vec{x}_4 \rangle &= V(\vec{x}_3, \vec{x}_4)\, \langle \vec{x}_1, \vec{x}_2 | \vec{x}_3, \vec{x}_4 \rangle \\ &= V(\vec{x}_1, \vec{x}_2)\, \delta^3(\vec{x}_1 - \vec{x}_3)\delta^3(\vec{x}_2 - \vec{x}_4) \end{aligned}$$

- general two-particle matrix elements:

$$\begin{aligned} \langle i, j, | \hat{f} | m, n \rangle &= \int d^3x_1 \ldots d^3x_4 \langle i | \vec{x}_1 \rangle \langle j | \vec{x}_2 \rangle \langle \vec{x}_1, \vec{x}_2 | \hat{f} | \vec{x}_3, \vec{x}_4 \rangle \langle \vec{x}_3 | m \rangle \langle \vec{x}_4 | n \rangle \\ &= \int d^3x_1 \ldots d^3x_4\, \varphi_i^*(\vec{x}_1)\, \varphi_j^*(\vec{x}_2)\, \langle \vec{x}_1, \vec{x}_2 | \hat{V}(\hat{\vec{x}}_{(1)}, \hat{\vec{x}}_{(2)}) | \vec{x}_3, \vec{x}_4 \rangle\, \varphi_m(\vec{x}_3)\, \varphi_n(\vec{x}_4) \\ &= \int d^3x_1 d^3x_2\, \varphi_i^*(\vec{x}_1)\, \varphi_j^*(\vec{x}_2)\, V(\vec{x}_1, \vec{x}_2)\, \varphi_m(\vec{x}_1)\, \varphi_n(\vec{x}_2) \end{aligned}$$

Summary

- Hamiltonian:

$$H = \sum_{\alpha} \left(\hat{t}_\alpha + \hat{U}(\hat{\vec{x}}_\alpha)\right) + \frac{1}{2} \sum_{\alpha \neq \beta} \hat{V}(\hat{\vec{x}}_\alpha, \hat{\vec{x}}_\beta)$$

$$= \sum_{ij} \left(t_{ij} + U_{ij}\right) a_i^\dagger a_j + \frac{1}{2} \sum_{ijmn} V_{ijmn}\, a_i^\dagger a_j^\dagger a_n a_m$$

- single-particle matrix elements:
  - $t_{ij} \equiv \langle i | \hat{t} | j \rangle$
  - $U_{ij} \equiv \langle i | \hat{U}(\hat{\vec{x}}) | j \rangle = \int d^3x\, \varphi_i^*(\vec{x})\, U(\vec{x})\, \varphi_j(\vec{x}),$

φ: single-particle wave function in position space

- two-particle matrix elements:
  - $V_{ijmn} \equiv \langle i, j | \hat{V}(\hat{\vec{x}}_{(1)}, \hat{\vec{x}}_{(2)},) | m, n \rangle$

$$= \int d^3x_1 d^3x_2\, \varphi_i^*(\vec{x}_1)\, \varphi_j^*(\vec{x}_2)\, V(\vec{x}_1, \vec{x}_2)\, \varphi_m(\vec{x}_1)\, \varphi_n(\vec{x}_2)$$