4.4 Field operators

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- two complete single-particle bases: $\{|i\rangle\}, \; \{|\lambda\rangle\}$
- basis change: $a^\dagger_\lambda |0\rangle = |\lambda\rangle = \sum_i |i\rangle\langle i|\lambda\rangle = \sum_i \langle i|\lambda\rangle a^\dagger_i |0\rangle$

$$\Rightarrow \; a^\dagger_\lambda = \sum_i \langle i|\lambda\rangle \, a^\dagger_i = \sum_i \langle \lambda|i\rangle^* \, a^\dagger_i \qquad \Rightarrow \; a_\lambda = \sum_i \langle \lambda|i\rangle \, a_i$$

- important case:

$\{|\lambda\rangle\} = \{|\vec{x}\rangle\}$ (position-space eigenstates), $\quad \langle \vec{x}|i\rangle = \varphi_i(\vec{x})$

→ "field operators": $\psi(\vec{x}) \equiv a_{\vec{x}} = \sum_i \varphi_i(\vec{x}) \, a_i$,

$$\psi^\dagger(\vec{x}) \equiv a^\dagger_{\vec{x}} = \sum_i \varphi^*_i(\vec{x}) \, a^\dagger_i$$

Interpretation

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- $\psi^\dagger(\vec{x})\,|0\rangle = \sum_i \varphi_i^*(\vec{x})\, a_i^\dagger\,|0\rangle = \sum_i |i\rangle\langle i|\vec{x}\rangle = |\vec{x}\rangle$
- particle number:

$$\hat{N}\,\psi^\dagger(\vec{x})\,|0\rangle = \sum_j a_j^\dagger a_j \sum_i \varphi_i^*(\vec{x})\, a_i^\dagger\,|0\rangle = \sum_{ij} \varphi_i^*(\vec{x})\, a_j^\dagger a_j a_i^\dagger\,|0\rangle$$

  - bosons: $a_j a_i^\dagger\,|0\rangle = \underbrace{[a_j, a_i^\dagger]}_{=\delta_{ji}}\,|0\rangle + a_i^\dagger\,\underbrace{a_j|0\rangle}_{=0} = \delta_{ji}\,|0\rangle$
  - fermions: $a_j a_i^\dagger\,|0\rangle = \underbrace{\{a_j, a_i^\dagger\}}_{=\delta_{ji}}\,|0\rangle - a_i^\dagger\,\underbrace{a_j|0\rangle}_{=0} = \delta_{ji}\,|0\rangle$

$$\Rightarrow \quad \hat{N}\,\psi^\dagger(\vec{x})\,|0\rangle = \sum_i \varphi_i^*(\vec{x})\, a_i^\dagger\,|0\rangle = \psi^\dagger(\vec{x})\,|0\rangle \quad \Rightarrow \quad N = 1$$

→ $\psi^\dagger(\vec{x})$ creates a particle at position $\vec{x}$.

Analogously, $\psi(\vec{x})$ annihilates a particle at position $\vec{x}$.

Commutator relations

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- Notation, allowing a common treatment of bosons and fermions:

$$\left[A, B\right]_\pm \equiv AB \pm BA \quad \Rightarrow \quad \left[A, B\right]_+ \equiv \{A, B\}, \quad \left[A, B\right]_- \equiv \left[A, B\right]$$

- $\left[\psi(\vec{x}), \psi(\vec{x}')\right]_\pm = \sum_{ij} \varphi_i(\vec{x})\varphi_j(\vec{x}') \underbrace{[a_i, a_j]_\pm}_{=0} = 0$

- analogously: $\left[\psi^\dagger(\vec{x}), \psi^\dagger(\vec{x}')\right]_\pm = 0$

- $\left[\psi(\vec{x}), \psi^\dagger(\vec{x}')\right]_\pm = \sum_{ij} \varphi_i(\vec{x})\varphi_j^*(\vec{x}') \underbrace{[a_i, a_j^\dagger]_\pm}_{=\delta_{ij}}$

$$= \sum_i \varphi_i(\vec{x})\varphi_i^*(\vec{x}') = \sum_i \langle \vec{x}|i\rangle\langle i|\vec{x}'\rangle = \langle \vec{x}|\vec{x}'\rangle = \delta^3(\vec{x} - \vec{x}')$$

$$\Rightarrow \quad \boxed{\left[\psi(\vec{x}), \psi(\vec{x}')\right]_\pm = \left[\psi^\dagger(\vec{x}), \psi^\dagger(\vec{x}')\right]_\pm = 0, \quad \left[\psi(\vec{x}), \psi^\dagger(\vec{x}')\right]_\pm = \delta^3(\vec{x} - \vec{x}')}$$

(+ for fermions, $-$ for bosones)

Single- and two-particle operators

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- kinetic energy:

$$\hat{T} = \sum_{ij} \langle i|\hat{t}|j\rangle\, a_i^\dagger a_j = \sum_{ij} \int d^3x \int d^3x' \, \underbrace{\langle i|\vec{x}'\rangle}_{\varphi_i^*(\vec{x}')} \langle \vec{x}'|\hat{t}|\vec{x}\rangle \underbrace{\langle \vec{x}|j\rangle}_{\varphi_j(\vec{x})} \, a_i^\dagger a_j$$

$$= \int d^3x \int d^3x' \, \psi^\dagger(\vec{x}')\, \langle \vec{x}'|\hat{t}|\vec{x}\rangle\, \psi(\vec{x})$$

$$\hat{t} = \frac{\hbar^2 \hat{\vec{k}}^2}{2m} \quad \Rightarrow \quad \langle \vec{x}'|\hat{t}|\vec{x}\rangle = \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \underbrace{\langle \vec{x}'|\vec{k}'\rangle}_{e^{i\vec{k}'\cdot\vec{x}'}} \quad \underbrace{\langle \vec{k}'|\hat{t}|\vec{k}\rangle}_{\frac{\hbar^2\vec{k}^2}{2m}(2\pi)^3\delta^3(\vec{k}'-\vec{k})} \quad \underbrace{\langle \vec{k}|\vec{x}\rangle}_{e^{-i\vec{k}\cdot\vec{x}}}$$

$$= \int \frac{d^3k}{(2\pi)^3} \, \frac{\hbar^2\vec{k}^2}{2m} \, e^{i\vec{k}\cdot(\vec{x}'-\vec{x})}$$

$$\Rightarrow \quad \hat{T} = \int d^3x \int d^3x' \int \frac{d^3k}{(2\pi)^3} \, \psi^\dagger(\vec{x}') \, \frac{\hbar^2\vec{k}^2}{2m} \, e^{i\vec{k}\cdot(\vec{x}'-\vec{x})} \psi(\vec{x})$$

$$\hat{T} = \int d^3x \int d^3x' \int \frac{d^3k}{(2\pi)^3}\, \psi^\dagger(\vec{x}')\, \frac{\hbar^2\vec{k}^2}{2m}\, e^{i\vec{k}\cdot(\vec{x}'-\vec{x})}\psi(\vec{x})$$

$$= \int d^3x \int d^3x' \int \frac{d^3k}{(2\pi)^3}\, \psi^\dagger(\vec{x}')\, \Big(-\frac{\hbar^2\vec{\nabla}^2}{2m}\, e^{i\vec{k}\cdot(\vec{x}'-\vec{x})}\Big)\psi(\vec{x})$$

integrate by parts twice:

$$= \int d^3x \int d^3x' \underbrace{\int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot(\vec{x}'-\vec{x})}}_{\delta^3(\vec{x}'-\vec{x})} \psi^\dagger(\vec{x}')\, (-\frac{\hbar^2\vec{\nabla}^2}{2m})\, \psi(\vec{x})$$

$$= -\frac{\hbar^2}{2m} \int d^3x \psi^\dagger(\vec{x})\, \vec{\nabla}^2\, \psi(\vec{x}) \overset{\text{int. by parts}}{=} \frac{\hbar^2}{2m} \int d^3x\, \Big(\vec{\nabla}\psi^\dagger(\vec{x})\Big) \cdot \Big(\vec{\nabla}\psi(\vec{x})\Big)$$

- single-particle potential:

$$\hat{U} = \sum_{ij} \langle i|\hat{U}(\hat{\vec{x}})|j\rangle\, a_i^\dagger a_j = \int d^3x \int d^3x'\, \psi^\dagger(\vec{x}')\, \underbrace{\langle \vec{x}'|\hat{U}(\hat{\vec{x}})|\vec{x}\rangle}_{U(\vec{x})\delta(\vec{x}'-\vec{x})}\, \psi(\vec{x})$$

$$= \int d^3x\, \psi^\dagger(\vec{x})\, U(\vec{x})\, \psi(\vec{x})$$

- two-particle operators:

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

$$= \frac{1}{2} \sum_{ijmn} \int d^3x_1 d^3x_2 \, \varphi_i^*(\vec{x}_1)\, \varphi_j^*(\vec{x}_2)\, V(\vec{x}_1,\vec{x}_2)\, \varphi_m(\vec{x}_1)\, \varphi_n(\vec{x}_2)\, a_i^\dagger a_j^\dagger a_n a_m$$

$$= \frac{1}{2} \int d^3x_1 d^3x_2 \, \psi^\dagger(\vec{x}_1)\, \psi^\dagger(\vec{x}_2)\, V(\vec{x}_1,\vec{x}_2)\, \psi(\vec{x}_2)\, \psi(\vec{x}_1)$$

→ Hamiltonian:

$$H = \int d^3x \left(\frac{\hbar^2}{2m} \big(\vec{\nabla}\psi^\dagger(\vec{x})\big) \cdot \big(\vec{\nabla}\psi(\vec{x})\big) \; + \; \psi^\dagger(\vec{x})\, U(\vec{x})\, \psi(\vec{x}) \right)$$

$$+ \frac{1}{2} \int d^3x_1 d^3x_2 \, \psi^\dagger(\vec{x}_1)\, \psi^\dagger(\vec{x}_2)\, V(\vec{x}_1,\vec{x}_2)\, \psi(\vec{x}_2)\, \psi(\vec{x}_1)$$

- particle density operator: $\hat{n}(\vec{x}) = \sum_\alpha \delta^3(\vec{x} - \hat{\vec{x}}_\alpha)$

$$\Rightarrow \hat{n}(\vec{x})|\vec{x}_1, \dots, \vec{x}_N\rangle = \sum_\alpha \delta^3(\vec{x} - \vec{x}_\alpha)|\vec{x}_1, \dots, \vec{x}_N\rangle$$

general single-particle operators: $\hat{T} = \sum_\alpha \hat{t}_\alpha = \sum_{ij} \langle i|\hat{t}|j\rangle \, a_i^\dagger a_j$

$$\Rightarrow \quad \hat{n}(\vec{x}) = \sum_{ij} \langle i|\delta^3(\underset{\substack{\uparrow \\ \text{“c number”}}}{\vec{x}} - \underset{\substack{\uparrow \\ \text{operator}}}{\hat{\vec{x}}})|j\rangle \, a_i^\dagger a_j$$

$$= \sum_{ij} \int d^3x' \int d^3x'' \langle i|\vec{x}''\rangle \underbrace{\langle \vec{x}''|\delta^3(\vec{x} - \hat{\vec{x}})|\vec{x}'\rangle}_{\delta^3(\vec{x}-\vec{x}')\,\delta^3(\vec{x}''-\vec{x}')} \langle \vec{x}'|j\rangle \, a_i^\dagger a_j$$

$$= \sum_{ij} \varphi_i^*(\vec{x})\, \varphi_j(\vec{x})\, a_i^\dagger a_j = \psi^\dagger(\vec{x})\psi(\vec{x})$$

$\Rightarrow$ total particle-number operator: $\hat{N} = \int d^3x \, \hat{n}(\vec{x}) = \int d^3x \, \psi^\dagger(\vec{x})\psi(\vec{x})$

Second quantization

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- $\hat{n}(\vec{x}) = \psi^\dagger(\vec{x})\psi(\vec{x})$, $\quad \hat{N} = \int d^3x\, \psi^\dagger(\vec{x})\psi(\vec{x})$:

  formal similarity with the probability density and the total probability in the Schrödinger theory

- Schrödinger: $\quad \psi(\vec{x})$ = wave function

  $\rightarrow$ $n(\vec{x})$ = function (classical field), N = number

- now: $\quad \psi(\vec{x})$ = operator $\;\rightarrow\;$ $\hat{n}(\vec{x})$, $\hat{N}$ = operators

This correspondence is called "second quantization".

- single-particle operators:
  - $\hat{T} = \int d^3x \psi^\dagger(\vec{x}) \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 \right) \psi(\vec{x})$
  - $\hat{U} = \int d^3x\, \psi^\dagger(\vec{x})\, U(\vec{x})\, \psi(\vec{x})$

  look like expectation values but are operators

Field equation

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- Heisenberg picture → time dependent field ops.: $\psi(\vec{x},t) = e^{\frac{i}{\hbar}Ht}\psi(\vec{x})e^{-\frac{i}{\hbar}Ht}$
- commutator relations at equal times:

$$\left[\psi(\vec{x},t),\psi(\vec{x}',t)\right]_{\pm} = \left[\psi^\dagger(\vec{x},t),\psi^\dagger(\vec{x}',t)\right]_{\pm} = 0, \quad \left[\psi(\vec{x},t),\psi^\dagger(\vec{x}',t)\right]_{\pm} = \delta^3(\vec{x}-\vec{x}')$$

- Heisenberg equation: $\frac{\partial}{\partial t}\psi(\vec{x},t) = \frac{1}{i\hbar}\left[\psi(\vec{x},t), H\right]$
- explicit evaluation for

$$H = \int d^3x\, \psi^\dagger(\vec{x},t)\Big(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{x})\Big)\psi(\vec{x},t)$$
$$+\frac{1}{2}\int d^3x_1 d^3x_2\, \psi^\dagger(\vec{x}_1,t)\,\psi^\dagger(\vec{x}_2,t)\, V(\vec{x}_1,\vec{x}_2)\,\psi(\vec{x}_2,t)\,\psi(\vec{x}_1,t)$$

→ form of a non-linear Schrödinger equation (see exercises):

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t) = \Big(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{x})\Big)\psi(\vec{x},t)$$
$$+\int d^3x'\, \psi^\dagger(\vec{x}',t)\, V(\vec{x},\vec{x}')\,\psi(\vec{x}',t)\,\psi(\vec{x},t)$$

4.5 Momentum representation

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- working in momentum space often more convenient (see scattering theory)
- single-particle basis: plane waves $\varphi_{\vec{k}}(\vec{x}) \propto e^{i\vec{k}\cdot\vec{x}}$
- simplification: finite volume + periodic boundary conditions
  - $V = L_x\, L_y\, L_z$,
  - $\varphi_{\vec{k}}(\vec{x}) = \varphi_{\vec{k}}(\vec{x} + L_x\vec{e}_x) = \varphi_{\vec{k}}(\vec{x} + L_y\vec{e}_y) = \varphi_{\vec{k}}(\vec{x} + L_z\vec{e}_z)$

  ➞ normalizable, discrete basis states $|\vec{k}\rangle$
- orthonormalized basis wave functions:

$$\langle\vec{x}|\vec{k}\rangle = \varphi_{\vec{k}}(\vec{x}) = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{x}}, \quad \vec{k} \in 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right), \quad n_i \in \mathbb{Z}$$

$$\Rightarrow \quad \langle\vec{k}'|\vec{k}\rangle = \int_V d^3x\ \varphi^*_{\vec{k}'}(\vec{x})\varphi_{\vec{k}}(\vec{x}) = \delta_{\vec{k}',\vec{k}}$$

- kinetic energy:

$$t_{\vec{k}',\vec{k}} = \langle \vec{k}' | \frac{\hbar^2 \hat{\vec{k}}^2}{2m} | \vec{k} \rangle = \frac{\hbar^2 \vec{k}^2}{2m} \langle \vec{k}' | \vec{k} \rangle = \frac{\hbar^2 \vec{k}^2}{2m} \delta_{\vec{k}',\vec{k}}$$

$$\Rightarrow \quad \hat{T} = \sum_{\vec{k}',\vec{k}} t_{\vec{k}',\vec{k}} \, a^\dagger_{\vec{k}'} a_{\vec{k}} = \sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m} \, a^\dagger_{\vec{k}} a_{\vec{k}} = \sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m} \, \hat{n}_{\vec{k}}$$

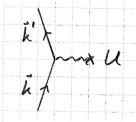
- single-particle potential:

$$U_{\vec{k}',\vec{k}} = \langle \vec{k}' | U(\hat{\vec{x}}) | \vec{k} \rangle = \int d^3x \int d^3x' \, \langle \vec{k}' | \vec{x}' \rangle \langle \vec{x}' | U(\hat{\vec{x}}) | \vec{x} \rangle \langle \vec{x} | \vec{k} \rangle$$

$$= \int d^3x \, \varphi^*_{\vec{k}'}(\vec{x}) \, U(\vec{x}) \, \varphi_{\vec{k}}(\vec{x}) = \frac{1}{V} \int d^3x \, e^{-i(\vec{k}' - \vec{k})\cdot\vec{x}} \, U(\vec{x}) = \frac{1}{V} \tilde{U}(\vec{k}' - \vec{k})$$

(Fourier transform)

$$\Rightarrow \quad \hat{U} = \frac{1}{V} \sum_{\vec{k}',\vec{k}} \tilde{U}(\vec{k}' - \vec{k}) \, a^\dagger_{\vec{k}'} a_{\vec{k}}$$



- two-particle potential: $\hat{V} = \frac{1}{2} \sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} V_{\vec{k}_3\vec{k}_4\vec{k}_1\vec{k}_2} \; a^\dagger_{\vec{k}_3} a^\dagger_{\vec{k}_4} a_{\vec{k}_2} a_{\vec{k}_1}$

$$V_{\vec{k}_3\vec{k}_4\vec{k}_1\vec{k}_2} = \int d^3x_1\, d^3x_2\; \varphi^*_{\vec{k}_3}(\vec{x}_1)\, \varphi^*_{\vec{k}_4}(\vec{x}_2)\, V(x_1, x_2)\, \varphi_{\vec{k}_1}(\vec{x}_1)\, \varphi_{\vec{k}_2}(\vec{x}_2)$$

$$= \frac{1}{V^2} \int d^3x_1\, d^3x_2\; e^{-i(\vec{k}_3-\vec{k}_1)\cdot\vec{x}_1}\, e^{-i(\vec{k}_4-\vec{k}_2)\cdot\vec{x}_2}\, V(x_1, x_2)$$

Invariance under translations:

V depends only on the relative coordinates: $V(\vec{x}_1, \vec{x}_2) = V(\vec{x}_1 - \vec{x}_2)$

Fourier transform: $\tilde{V}(\vec{q}) = \int d^3x\, e^{-i\vec{q}\cdot\vec{x}} V(\vec{x}) \;\Leftrightarrow\; V(\vec{x}) = \frac{1}{V} \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{x}}\, \tilde{V}(\vec{q})$

$$\Rightarrow\quad V_{\vec{k}_3\vec{k}_4\vec{k}_1\vec{k}_2} = \frac{1}{V^3} \sum_{\vec{q}} \tilde{V}(\vec{q}) \int d^3x_1\, d^3x_2\; e^{-i(\vec{k}_3-\vec{k}_1-\vec{q})\cdot\vec{x}_1}\, e^{-i(\vec{k}_4-\vec{k}_2+\vec{q})\cdot\vec{x}_2}$$

$$= \frac{1}{V} \sum_{\vec{q}} \tilde{V}(\vec{q})\, \delta_{\vec{k}_3,\vec{k}_1+\vec{q}}\, \delta_{\vec{k}_4,\vec{k}_2-\vec{q}}$$

$$\Rightarrow\quad \hat{V} = \frac{1}{2V} \sum_{\vec{k}_1,\vec{k}_2,\vec{q}} \tilde{V}(\vec{q})\; a^\dagger_{\vec{k}_1+\vec{q}}\, a^\dagger_{\vec{k}_2-\vec{q}}\, a_{\vec{k}_2}\, a_{\vec{k}_1}$$