Second quantization

Владимир Александрович Фок
(10/22.12. 1898 - 27.12.1974)

① States and elementary operators

- Fock space for identical particles

  - single-particle states $\alpha, \beta, \gamma \dots$ with the wavefunctions $\phi_\alpha, \phi_\beta, \phi_\gamma \dots$

  - Hilbert space of n-particle states $\mathcal{H}_n$

    basis states $|n_\alpha n_\beta n_\gamma \dots\rangle$ $\qquad n_\alpha + n_\beta + n_\gamma + \dots = n$

    ↑ number of particles in state α

    corresponds to symmetrized / antisymmetrized (bosons / fermions) product wf

$$\Psi(1,2,3,\dots,n) = \underbrace{\phi_\alpha(1)\,\phi_\alpha(2)\dots}_{n_\alpha \text{ terms}}\,\phi_\beta(n_\alpha+1)\dots$$

  - Fock space $\mathcal{F} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots$

- creation/annihilation operators and Fock states

$\hat{c}^+_\alpha$ creates particle in state α

$\hat{c}_\alpha$ removes particle in state α

Fock state

$|n_\alpha\, n_\beta\, n_\gamma\, n_\delta \ldots\rangle$

correspondence $\quad c^+_\alpha\, c^+_\beta\, c^+_\delta\, |vac\rangle \longleftrightarrow |1\ 1\ 0\ 1 \ldots\rangle$ Fermions

$b^+_\alpha\, b^+_\beta\, b^+_\beta\, b^+_\delta\, |vac\rangle \longleftrightarrow |1\ 2\ 1\ 0 \ldots\rangle$ bosons

commutation relations

Fermions $\quad \{c_\alpha, c_\beta\} = 0 \qquad \{c^+_\alpha, c^+_\beta\} = 0 \qquad \{c_\alpha, c^+_\beta\} = \delta_{\alpha\beta}$

$c^+_\alpha c^+_\beta = -c^+_\beta c^+_\alpha$ (antisymmetry) $\qquad c^+_\alpha\, c^+_\alpha = 0$ (Pauli principle)

bosons $\quad [b_\alpha, b_\beta] = 0 \qquad [b^+_\alpha, b^+_\beta] = 0 \qquad [b_\alpha, b^+_\beta] = \delta_{\alpha\beta}$

- examples for Fermions

1) three spinless Fermions

Slater determinant

$$c^+_\alpha c^+_\beta c^+_\gamma |vac\rangle \longleftrightarrow \Psi(1,2,3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \phi_\alpha(1) & \phi_\beta(1) & \phi_\gamma(1) \\ \phi_\alpha(2) & \phi_\beta(2) & \phi_\gamma(2) \\ \phi_\alpha(3) & \phi_\beta(3) & \phi_\gamma(3) \end{vmatrix}$$

2) singlet electron pair in a doubly occupied orbital

$$c^+_{\alpha\uparrow} c^+_{\alpha\downarrow} |vac\rangle = \text{antisymmetrized } \phi_\alpha(\bar{r}_1)\chi_\uparrow(\sigma_1)\, \phi_\alpha(\bar{r}_2)\chi_\downarrow(\sigma_2)$$

$$= \phi_\alpha(\bar{r}_1)\,\phi_\alpha(\bar{r}_2)\,\frac{1}{\sqrt{2}}\left[\chi_\uparrow(\sigma_1)\chi_\downarrow(\sigma_2) - \chi_\downarrow(\sigma_1)\chi_\uparrow(\sigma_2)\right]$$

3) triplet electron pair

$$c^+_{\alpha\uparrow} c^+_{\beta\uparrow} |vac\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_\alpha(\bar{r}_1)\chi_\uparrow(\sigma_1) & \phi_\beta(\bar{r}_1)\chi_\uparrow(\sigma_1) \\ \phi_\alpha(\bar{r}_2)\chi_\uparrow(\sigma_2) & \phi_\beta(\bar{r}_2)\chi_\uparrow(\sigma_2) \end{vmatrix} =$$

$$= \frac{1}{\sqrt{2}}\left[\phi_\alpha(\bar{r}_1)\phi_\beta(\bar{r}_2) - \phi_\beta(\bar{r}_1)\phi_\alpha(\bar{r}_2)\right]\chi_\uparrow(\sigma_1)\chi_\uparrow(\sigma_2)$$

4) singlet electron pair in two different orbitals

$$\frac{1}{\sqrt{2}}\left(c^+_{\alpha\uparrow}c^+_{\beta\downarrow} - c^+_{\alpha\downarrow}c^+_{\beta\uparrow}\right)|vac\rangle = \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}\begin{vmatrix}\alpha_\uparrow(1) & \beta_\downarrow(1)\\ \alpha_\uparrow(2) & \beta_\downarrow(2)\end{vmatrix} - \frac{1}{\sqrt{2}}\begin{vmatrix}\alpha_\downarrow(1) & \beta_\uparrow(1)\\ \alpha_\downarrow(2) & \beta_\uparrow(2)\end{vmatrix}\right]$$

$$= \frac{1}{2}\left[\alpha_\uparrow(1)\beta_\downarrow(2) - \beta_\downarrow(1)\alpha_\uparrow(2) - \alpha_\downarrow(1)\beta_\uparrow(2) + \beta_\uparrow(1)\alpha_\downarrow(2)\right]$$

$$= \frac{1}{\sqrt{2}}\left[\phi_\alpha(\bar{r}_1)\phi_\beta(\bar{r}_2) + \phi_\beta(\bar{r}_1)\phi_\alpha(\bar{r}_2)\right]\frac{1}{\sqrt{2}}\left[\chi_\uparrow(\sigma_1)\chi_\downarrow(\sigma_2) - \chi_\downarrow(\sigma_1)\chi_\uparrow(\sigma_2)\right]$$

- Field operators

Field operator $\hat{\psi}(\bar{r})$ removes particle at $\bar{r}$ $\rightarrow$ $|\bar{r}\rangle = \hat{\psi}^+(\bar{r})|vac\rangle$

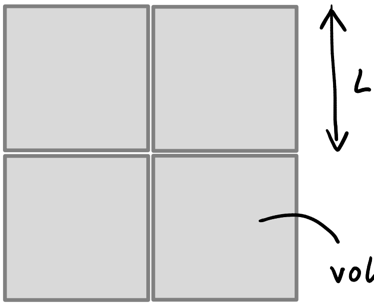
consider single-particle state $|\psi\rangle = \sum_\alpha w_\alpha \hat{c}^+_\alpha |vac\rangle$ with $\psi(\bar{r}) = \sum_\alpha w_\alpha \phi_\alpha(\bar{r})$

wave function $\psi(\bar{r})$ also obtained as

$$\psi(\bar{r}) = \langle \bar{r}|\psi\rangle = \langle vac|\hat{\psi}(\bar{r})|\psi\rangle \quad \begin{array}{l}\nearrow \quad \hat{\psi}(\bar{r}) = \sum_\alpha \phi_\alpha(\bar{r})\,\hat{c}_\alpha \\[1em] \searrow \quad \hat{\psi}^+(\bar{r}) = \sum_\alpha \phi^*_\alpha(\bar{r})\,\hat{c}^+_\alpha\end{array}$$

- normalization and Born-von Kármán cell

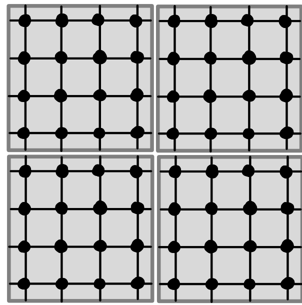
continuum



volume $\Omega = L^3$

(3D)

lattice version



number of sites $N = N_x N_y$

(2D)

Tight-binding picture:

$\hat{c}_{\bar{R}}$ associated with localized $\phi_{\bar{R}}(\bar{r})$

$$\{\hat{c}_{\bar{R}}, \hat{c}^{+}_{\bar{R}'}\} = \delta_{\bar{R},\bar{R}'}$$

- plane-wave basis

$$\phi_{\bar{k}}(\bar{r}) = \frac{e^{i\bar{k}\cdot\bar{r}}}{\sqrt{\Omega}} \qquad \bar{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$$

orthogonality

$$\int d^3\bar{r}\; \phi^*_{\bar{k}}(\bar{r})\,\phi_{\bar{k}'}(\bar{r}) = \delta_{\bar{k},\bar{k}'}$$

$$\{\hat{c}_{\bar{k}}, \hat{c}^{+}_{\bar{k}'}\} = \delta_{\bar{k},\bar{k}'}$$

- Bloch waves

$$|k\rangle = \hat{c}^{+}_{k}\,|vac\rangle = \frac{1}{\sqrt{N}} \sum_{\bar{R}} e^{i\bar{k}\cdot\bar{R}}\, \hat{c}^{+}_{\bar{R}}\,|vac\rangle$$

$$\rightarrow \quad \hat{c}_{\bar{R}} = \frac{1}{\sqrt{N}} \sum_{\bar{k}} e^{i\bar{k}\cdot\bar{R}}\, \hat{c}_{\bar{k}} \qquad \bar{k} = \frac{2\pi}{a}\left(\frac{n_x}{N_x}, \frac{n_y}{N_y}\right)$$

$$\hat{c}^{+}_{R} = \frac{1}{\sqrt{N}} \sum_{\bar{k}} e^{-i\bar{k}\cdot\bar{R}}\, \hat{c}^{+}_{k}$$

$n_x \in 0, 1, 2 \ldots N_x - 1$

$n_y \in 0, 1, 2 \ldots N_y - 1$

② Single-particle operators

$\hat{O} = \sum_n O_1(\bar{r}_n, \frac{\hbar}{i}\nabla_{\bar{r}_n}, \hat{\bar{S}}_n)$ position, momentum & spin of particle n

recipe using field operators $\hat{O} = \int d^3\bar{r} \sum_{\sigma\sigma'} \hat{\psi}^+_\sigma(\bar{r})\, O_1(\bar{r}, \frac{\hbar}{i}\nabla, \hat{\bar{S}})\, \hat{\psi}_{\sigma'}(\bar{r})$

- density at point $\bar{r}$: $\hat{n}(\bar{r}) = \sum_j \delta(\bar{r} - \hat{\bar{r}}_j)$

$$\rightarrow \hat{n}(\bar{r}) = \int d^3\bar{r}' \sum_{\sigma\sigma'} \hat{\psi}^+_\sigma(\bar{r}')\, \delta(\bar{r}-\bar{r}')\, \delta_{\sigma\sigma'}\, \hat{\psi}_{\sigma'}(\bar{r}') = \sum_\sigma \hat{\psi}^+_\sigma(\bar{r})\hat{\psi}_\sigma(\bar{r})$$

$$= \frac{1}{\sqrt{\Omega}^2} \sum_{kk'\sigma} e^{-i\bar{k}\cdot\bar{r}} e^{i\bar{k}'\cdot\bar{r}}\, \hat{c}^+_{k\sigma}\hat{c}_{k'\sigma} = \frac{1}{\Omega}\sum_{kq\sigma} e^{i\bar{q}\cdot\bar{r}}\, \hat{c}^+_{k\sigma}\hat{c}_{k+q,\sigma}$$

- total number $\hat{N} = \int d^3\bar{r}\, \hat{n}(\bar{r}) = \sum_{k\sigma} \hat{c}^+_{k\sigma}\hat{c}_{k\sigma}$

- kinetic energy $\hat{T} = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m}\hat{c}^+_{k\sigma}\hat{c}_{k\sigma}$

- Fourier component of $\hat{n}$ defined via $\hat{n}(\bar{r}) = \sum_{\bar{q}} e^{i\bar{q}\cdot\bar{r}} \hat{n}_{\bar{q}}$

→ $\hat{n}_{\bar{q}}$ corresponds to the real amplitude of density modulation with the wavevector $\bar{q}$

$$\hat{n}_{\bar{q}} = \frac{1}{\Omega}\int d^3\bar{r}\, e^{-i\bar{q}\cdot\bar{r}}\, \hat{n}(\bar{r}) = \frac{1}{\Omega^2}\sum_{kq'G} \underbrace{\int d^3\bar{r}\, e^{-i\bar{q}\cdot\bar{r}}\, e^{i\bar{q}'\cdot\bar{r}}}_{\Omega\,\delta_{\bar{q},\bar{q}'}} \hat{c}^+_{kG}\, \hat{c}_{k+q',G} = \frac{1}{\Omega}\sum_{kG} \hat{c}^+_{kG}\, \hat{c}_{k+q,G}$$

- coupling to external potential (for electrons)

charge density $\hat{\rho}(\bar{r}) = (-e)\sum_{q} e^{i\bar{q}\cdot\bar{r}}\, \hat{n}_{\bar{q}}$

electrostatic potential $\varphi(\bar{r}) = \sum_{q} e^{i\bar{q}\cdot\bar{r}}\, \varphi_{\bar{q}}$

coupling $\hat{H}_{int} = \int d^3\bar{r}\, \varphi(\bar{r})\,\hat{\rho}(\bar{r}) = (-e)\sum_{q}\sum_{q'} \int d^3\bar{r}\, e^{i\bar{q}\cdot\bar{r}}\varphi_{\bar{q}}\, e^{i\bar{q}'\cdot\bar{r}}\, \hat{n}_{\bar{q}'}$

$$= \Omega \sum_{q} (-e)\, \hat{n}_{-q}\, \varphi_{q}$$

lattice operators:

- site occupation $\hat{n}_R = \sum_\sigma \hat{c}^+_{R\sigma} \hat{c}_{R\sigma} = \frac{1}{N} \sum_{kq\sigma} e^{i\bar{q}\cdot\bar{R}} \hat{c}^+_{k\sigma} \hat{c}_{k+q,\sigma}$

  average site occupation $\hat{n} = \frac{1}{N} \sum_R \hat{n}_R = \frac{1}{N^2} \sum_{kq\sigma} \underbrace{\sum_R e^{i\bar{q}\cdot\bar{R}}}_{N\delta_{\bar{q},\bar{0}}} \hat{c}^+_{k\sigma} \hat{c}_{k+q,\sigma} = \frac{1}{N} \sum_{k\sigma} \hat{c}^+_{k\sigma} \hat{c}_{k\sigma}$

- tight-binding Hamiltonian

$$\hat{H} = -t \sum_{R\sigma} \sum_\delta \hat{c}^+_{R\sigma} \hat{c}_{R+\delta,\sigma} = -t \frac{1}{N} \sum_{kk'\sigma} \sum_\delta \sum_R e^{-i\bar{k}\cdot\bar{R}} e^{i\bar{k}'\cdot(\bar{R}+\bar{\delta})} \hat{c}^+_{k\sigma} \hat{c}_{k'\sigma}$$

$$= -t \sum_{k\sigma} \sum_\delta e^{i\bar{k}\cdot\bar{\delta}} \hat{c}^+_{k\sigma} \hat{c}_{k\sigma} = \sum_{k\sigma} \varepsilon_k \hat{c}^+_{k\sigma} \hat{c}_{k\sigma} \quad \text{with} \quad \varepsilon_k = -t \sum_\delta e^{i\bar{k}\cdot\bar{\delta}}$$

- α-component of electron spin

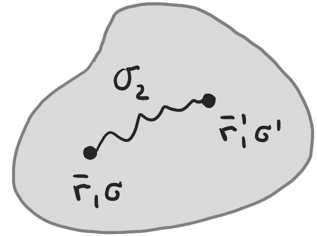
$$\hat{S}^\alpha_R = \frac{1}{N} \sum_{kss'} e^{i\bar{q}\cdot\bar{R}} \hat{c}^+_{ks} \frac{1}{2} \sigma^\alpha_{ss'} \hat{c}_{k+q\,s'} \qquad \sigma^\alpha \text{ ... Pauli matrix}$$

$$\hat{S}^z_R = \frac{1}{2}(\hat{n}_{R\uparrow} - \hat{n}_{R\downarrow}) = \frac{1}{N} \sum_{k\sigma} e^{i\bar{q}\cdot\bar{R}} \frac{1}{2}(\hat{c}^+_{k\uparrow} \hat{c}_{k+q\uparrow} - \hat{c}^+_{k\downarrow} \hat{c}_{k+q\downarrow})$$

③ Two-particle operators

$$\hat{\sigma} = \sum_{n<n'} \sigma_2\left(\bar{r}_n, \bar{r}_{n'}, \frac{\hbar}{i}\nabla_{\bar{r}_n}, \frac{\hbar}{i}\nabla_{\bar{r}_{n'}}, \hat{\bar{S}}_n, \hat{\bar{S}}_{n'}\right) = \frac{1}{2}\sum_{n\neq n'} \sigma_2(\dots)$$

(self-interaction excluded, each pair included once)



$$\hat{\sigma} = \frac{1}{2}\int d^3\bar{r}\int d^3\bar{r}' \sum_{GG'} \hat{\psi}^+_G(\bar{r})\,\hat{\psi}^+_{G'}(\bar{r}')\,\sigma_2(\bar{r},\bar{r}',\dots)\,\hat{\psi}_{G'}(\bar{r}')\,\hat{\psi}_G(\bar{r})$$ (spin-independent)

- Coulomb interaction in electron gas

$$\sigma_2(\bar{r},\bar{r}') = \frac{e^2}{4\pi\varepsilon_0|\bar{r}-\bar{r}'|} \qquad \hat{\psi}_G(\bar{r}) = \frac{1}{\sqrt{\Omega}}\sum_{\bar{k}} e^{i\bar{k}\cdot\bar{r}}\,\hat{c}_{\bar{k}G}$$

$$\hat{V}_{coul} = \frac{1}{2}\sum_{k_1\dots k_4}\sum_{GG'} \frac{1}{\Omega^2}\int d^3\bar{r}'\int d^3\bar{r}''\, e^{-i\bar{k}_1\cdot\bar{r}'} e^{-i\bar{k}_2\cdot\bar{r}''} e^{i\bar{k}_3\cdot\bar{r}''} e^{i\bar{k}_4\cdot\bar{r}'} \times$$

$$\times \frac{e^2}{4\pi\varepsilon_0|\bar{r}'-\bar{r}''|}\,\hat{c}^+_{k_1G}\,\hat{c}^+_{k_2G'}\,\hat{c}_{k_3G'}\,\hat{c}_{k_4G}$$

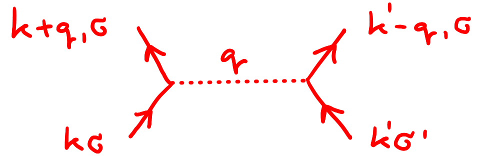
$$e^{-i\bar{k}_1\cdot\bar{r}'}e^{-i\bar{k}_2\cdot\bar{r}''}e^{i\bar{k}_3\cdot\bar{r}''}e^{i\bar{k}_4\cdot\bar{r}'} \xrightarrow{\bar{r}'-\bar{r}''=\bar{r}} e^{-i\bar{k}_1\cdot(\bar{r}+\bar{r}'')}e^{-i\bar{k}_2\cdot\bar{r}''}e^{i\bar{k}_3\cdot\bar{r}''}e^{i\bar{k}_4\cdot(\bar{r}+\bar{r}'')}$$

$$= e^{i(-\bar{k}_1-\bar{k}_2+\bar{k}_3+\bar{k}_4)\cdot\bar{r}''}\, e^{i(\bar{k}_4-\bar{k}_1)\cdot\bar{r}}$$

$\int d^3\bar{r}''$ gives $\Omega\,\delta_{-\bar{k}_1-\bar{k}_2+\bar{k}_3+\bar{k}_4,\bar{0}}$

$\rightarrow \quad k_1 = k+q\,,\quad k_2 = k'-q\,,\quad k_3 = k'\,,\quad k_4 = k$

$\int d^3\bar{r}$ gives



$$\hat{V}_{coul} = \frac{1}{2}\sum_{kk'q}\sum_{\sigma\sigma'} V_{\bar{q}}\,\hat{c}^+_{k+q\,\sigma}\,\hat{c}^+_{k'-q\,\sigma'}\,\hat{c}_{k'\sigma'}\,\hat{c}_{k\sigma} \qquad V_{\bar{q}} = \frac{1}{\Omega}\int d^3\bar{r}\; e^{-i\bar{q}\cdot\bar{r}}\,\frac{e^2}{4\pi\varepsilon_0 r} = \frac{1}{\Omega}\,\frac{e^2}{\varepsilon_0 q^2}$$

- Hubbard interaction on a lattice ○ (↑) (↓) (↑↓)

U

$$\hat{H}_U = U\sum_R \hat{n}_{R\uparrow}\hat{n}_{R\downarrow} = U\sum_R \frac{1}{N^2}\sum_{kq} e^{-i\bar{q}\cdot\bar{R}}\,\hat{c}^+_{k+q\uparrow}\,\hat{c}_{k\uparrow}\sum_{k'q'} e^{-i\bar{q}'\cdot\bar{R}}\,\hat{c}^+_{k'+q'\downarrow}\,\hat{c}_{k'\downarrow}$$

using density op.: $\hat{n}_{R\sigma} = \frac{1}{N}\sum_{kq} e^{i\bar{q}\cdot\bar{R}}\,\hat{c}^+_{k\sigma}\,\hat{c}_{k+q,\sigma} = \frac{1}{N}\sum_{kq} e^{-i\bar{q}\cdot R}\,\hat{c}^+_{k+q\sigma}\,\hat{c}_{k\sigma}$

$$= U\,\frac{1}{N}\sum_{kk'q}\hat{c}^+_{k+q\uparrow}\,\hat{c}^+_{k'-q\downarrow}\,\hat{c}_{k'\downarrow}\,\hat{c}_{k\uparrow}$$

local interaction → q-independent