Properties: $u_{\vec{p}} = u_{-\vec{p}}$, $v_{\vec{p}} = v_{-\vec{p}}$

$$|u_{\vec{p}}|^2 - |v_{\vec{p}}|^2 = 1 .$$

Can show: $[\hat{b}_{\vec{p}}, \hat{b}_{\vec{q}}] = [\hat{b}^+_{\vec{p}}, \hat{b}^+_{\vec{q}}] = 0$

$$[\hat{b}_{\vec{p}}, \hat{b}^+_{\vec{q}}] = \delta_{\vec{p},\vec{q}}$$

Rewrite $\hat{H}$ in new basis (choose $u, v \in \mathbb{R}$):

$$\hat{H} = \frac{N^2}{2V} \tilde{U}_0^{(2)} + \sum_{\vec{p}}{}' u_{\vec{p}} \left(u_{\vec{p}} \frac{p^2}{2m} + (u_{\vec{p}} - v_{\vec{p}}) \frac{N}{V} \tilde{U}(\vec{p}) \right) \hat{b}^+_{\vec{p}} \hat{b}_{\vec{p}}$$

$$+ \sum_{\vec{p}}{}' v_{\vec{p}} \left(v_{\vec{p}} \frac{p^2}{2m} + (v_{\vec{p}} - u_{\vec{p}}) \frac{N}{V} \tilde{U}(\vec{p}) \right) \hat{b}_{\vec{p}} \hat{b}^+_{\vec{p}}$$

$$+ \sum_{\vec{p}}{}' \left(-u_{\vec{p}} v_{\vec{p}} \frac{p^2}{2m} + \frac{1}{2} (u_{\vec{p}} - v_{\vec{p}}) \frac{N}{V} \tilde{U}(\vec{p}) \right) \left(\hat{b}^+_{\vec{p}} \hat{b}^+_{-\vec{p}} + \hat{b}_{\vec{p}} \hat{b}_{-\vec{p}} \right)$$

Want to make last term vanish (Ansatz:)

$$\left(u_{\vec{p}} = \cosh(f(p^2)) \quad , \quad v_{\vec{p}} = \sinh(f(p^2)) \right)$$

satisfies symmetry and normalisation.

Solve $\quad u_p v_p \frac{p^2}{2m} - \frac{1}{2} (u_p - v_p)^2 \frac{N}{V} \tilde{U}(\vec{p}) = 0 \quad , \quad u_p^2 - v_p^2 = 1$

$$\Leftrightarrow \quad u_p^2 (u_p^2 - 1) = \frac{1}{4} \frac{1}{E_p^2} \left(\frac{N}{V} \tilde{U}(\vec{p}) \right)^2$$

$$\text{with} \quad E_p^2 = \frac{p^2}{2m} \left(\frac{p^2}{2m} + 2 \frac{N}{V} \tilde{U}(\vec{p}) \right)$$

$$\Rightarrow \quad u_p^2 = \frac{1}{2E_p} \left(\frac{p^2}{2m} + \frac{N}{V} \tilde{U}(\vec{p}) + E_p \right)$$

$$v_p^2 = \frac{1}{2E_p} \left(\frac{p^2}{2m} + \frac{N}{V} \tilde{U}(\vec{p}) - E_p \right)$$

Insert in $\hat{H}$; using $\hat{b}_{\vec{p}} \hat{b}^{+}_{\vec{p}} = \hat{b}^{+}_{\vec{p}} \hat{b}_{\vec{p}} + 1$:

$$\hat{H} = \frac{N^2}{2V} \tilde{V}_0 + \frac{1}{2} \sum_{\vec{p}}{}' \left(E_{\vec{p}} - \frac{p^2}{2m} - \frac{N}{V} \tilde{V}(\vec{p}) \right) + \sum_{\vec{p}}{}' E_{\vec{p}} \hat{b}^{+}_{\vec{p}} \hat{b}_{\vec{p}}$$

Diagonal Hamiltonian with ground state energy

$$E_0 = \frac{N^2}{2V} \tilde{V}_0 + \frac{1}{2} \sum_{\vec{p}}{}' \left(E_{\vec{p}} - \frac{p^2}{2m} - \frac{N}{V} \tilde{V}(\vec{p}) \right)$$

+ sum of harmonic oscillators with energies $E_{\vec{p}}$.

The states created by $\hat{b}^{+}_{\vec{p}}$ are often called <u>quasi-particles</u>.
They are different from the free particle states generated by $\hat{a}^{+}_{\vec{p}}$.

Ground state:

$$\hat{b}_{\vec{p}} | \Psi_0 \rangle = 0 \quad \forall \vec{p} \neq 0 .$$

Note: This is not the same state as the state where all particles have $\vec{p} = \vec{0}$ (ground state of non-interacting system).

Properties:

$$\sum_{\vec{p}}{}' \langle \Psi_0 | \hat{b}^{+}_{\vec{p}} \hat{b}_{\vec{p}} | \Psi_0 \rangle = 0 \quad \text{, i.e. no quasi-part.}$$

but

$$\sum_{\vec{p}}{}' \langle \Psi_0 | \hat{a}^{+}_{\vec{p}} \hat{a}_{\vec{p}} | \Psi_0 \rangle = \sum_{\vec{p}}{}' v_p^2 \langle \Psi_0 | \hat{b}_{\vec{p}} \hat{b}^{+}_{\vec{p}} | \Psi_0 \rangle$$

$$= \sum_{\vec{p}}{}' v_p^2 \neq 0 .$$

Consider a contact interaction, $V^{(2)}(\vec{x}_1 - \vec{x}_2) = \delta^3(\vec{x}_1 - \vec{x}_2)\,\lambda$.

$$\Rightarrow \quad \tilde{V}(\vec{p}) = \lambda .$$

Compute # particles not in $\vec{p}=0$ state:

$$N' = \sum_{\vec{p}}{}' \, v_{\vec{p}}^2 = \frac{V}{3\pi^2}\, m^{3/2} \left(\lambda \frac{N}{V}\right)^{3/2}$$

Note: $\left(\lambda \frac{N}{V}\right)$ is the expansion parameter; our initial assumption, that $N_{\vec{p}} \ll N \;\; \forall \vec{p} \neq 0$ becomes invalid for too large (λn).

The result is not analytic for $\lambda \to 0$, Can't find this result in perturbation theory.

Properties of quasi-particles:

small $\vec{p}$, have: $\quad E_{\vec{p}} = \sqrt{\frac{p^2}{2m}\left(\frac{p^2}{2m} + 2\frac{N}{V}\tilde{V}(\vec{p})\right)} \approx |\vec{p}|\sqrt{\frac{N\tilde{V}(\vec{p})}{Vm}}$

$$= v_{quasi}\, |\vec{p}|$$

Linear dispersion relation $\rightarrow$ <u>Phonon</u>

The system we described is called a Bose-Einstein condensate.

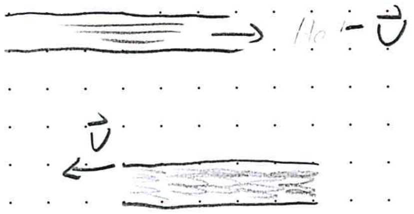
Suprafluidity (3.1.3)

At low temperatures, some liquids (e.g. Helium 4) are known to flow frictionless. We try to understand this in QM.

Consider He^4 flowing through a tube. Two frames of reference:

Laboratory system K

He rest frame K'



Frame K : E total energy of He

$\vec{P}$ total momentum

Frame K' : E' , $\vec{P}'$

Have : $E = E' - \vec{v}\vec{P}' + \frac{1}{2} M \vec{v}^2$

M: total mass

$P = \vec{P}' - M\vec{v}$

Consider first the frame K. Friction is described microscopically via scatterings of He-atoms with the wall. Loss of kinetic energy, transfer to wall.

$$\Rightarrow \quad \Delta E \leq 0 \quad \text{for scatterings}$$

Now in frame K'.

Assume that initially He is in ground state $|\Psi_0\rangle$, i.e. no phonon excitations.

Note: At low T, and for small momenta, the He^4 excitations satisfy

$$\epsilon_{\vec{p}} = v_{phonon} |\vec{p}| .$$

In ground state (initial state):

$$E_i' = E_0' \qquad \vec{P}_i' = \vec{0}$$

$$\Rightarrow \quad E_i = E_0' + \frac{1}{2} M\vec{v}^2 , \quad \vec{P}_i = -M\vec{v}$$

Friction excites quasiparticles in He that move along with the tube.
Consider excitation of single phonon with momentum $\vec{p}'$.

$$\Rightarrow \quad E_f' = E_0' + v_{phonon} |\vec{p}'|$$
$$\vec{P}_f' = \vec{p}'$$

and

$$E_f = E_0' + v_{phonon} |\vec{p}'| - \vec{v}\,\vec{p}' + \frac{1}{2} M\vec{v}^2$$
$$\vec{P}_f = \vec{p}' - M\vec{v}$$

$$\Rightarrow \quad \Delta E = E_f - E_i = v_{phonon} |\vec{p}'| - \vec{v}\,\vec{p}'$$

this satisfies $\Delta E < 0$ only if $|\vec{v}| > v_{phonon}$. For $|\vec{v}| < v_{phonon}$ there is no energy loss from friction.

Note: For larger $\vec{p}'$ the disp. rel. deviates from linear behavior
↳ suprafluidity for $|\vec{v}| < v_{crit}$, $v_{crit} < v_{phonon}$

Experimentally: $v_{crit} \approx 60 \frac{m}{s}$.

Breakdown corresponds to excitation of rotons

Fermions

Pauli principle → ground state will look different!

N spin $\frac{1}{2}$ particles in volume V, spin quantum number $\sigma = \pm\frac{1}{2}$.

$$\hat{a}_{\vec{p},\sigma} \; ; \; \hat{a}^{\dagger}_{\vec{p},\sigma} \; ; \quad \langle \vec{p},\sigma | \vec{q},\tau \rangle = \delta_{\vec{p},\vec{q}} \, \delta_{\sigma,\tau}$$

with the usual anti-comm. relations. Finally

$$\langle \vec{x},\sigma | \vec{p},\tau \rangle = \frac{1}{\sqrt{V}} e^{i\vec{p}\vec{x}} \delta_{\sigma\tau}$$

Free fermions

PP: Fill N-lowest energy states in ground state. The threshold is called Fermi-momentum p_F

$$|\Psi_0\rangle = \prod_{|\vec{p}| \le p_F} \prod_{\sigma} \hat{a}^{\dagger}_{\vec{p},\sigma} |0\rangle$$

$$N_{\vec{p},\sigma} = \langle \Psi_0 | \hat{a}^{\dagger}_{\vec{p},\sigma} \hat{a}_{\vec{p},\sigma} | \Psi_0 \rangle = \begin{cases} 1 & |\vec{p}| \le p_F \\ 0 & |\vec{p}| > p_F \end{cases}$$

Total particle #

$$N = \sum_{\vec{p}} \sum_{\sigma} \langle \Psi_0 | \hat{a}^{+}_{\vec{p},\sigma} \hat{a}_{\vec{p},\sigma} | \Psi_0 \rangle$$

$$= 2 \sum_{|\vec{p}| \leq p_F} 1 \approx \frac{2V}{(2\pi)^3} \int_{|\vec{p}| \leq p_F} d^3p = \frac{V p_F^3}{3\pi^2}$$

$$\Rightarrow \quad p_F^3 = 3\pi^2 \frac{N}{V}$$

Density in position space:

$$n_\psi = \sum_{\sigma} \langle \Psi_0 | \hat{\phi}^{+}_{\sigma}(x) \hat{\phi}_{\sigma}(x) | \Psi_0 \rangle$$

$$= \frac{1}{V} \sum_{\sigma} \sum_{\vec{p}, \vec{q}} e^{-i(\vec{p}-\vec{q})\vec{x}} \langle \Psi_0 | \hat{a}^{+}_{\vec{p},\sigma} \hat{a}_{\vec{q},\sigma} | \Psi_0 \rangle$$

$$= \frac{N}{V} \quad \longrightarrow \text{position independent}$$

2-point correlation:

$$\left(\frac{n_\psi}{2}\right)^2 g_{\sigma_1 \sigma_1}(\vec{x}_1, \vec{x}_2) = \langle \Psi | \hat{\phi}^{+}_{\sigma_1}(x_1) \hat{\phi}^{+}_{\sigma_2}(x_2) \hat{\phi}_{\sigma_2}(x_2) \hat{\phi}_{\sigma_1}(x_1) | \Psi \rangle$$

$$= \frac{1}{V^2} \sum_{\substack{\vec{p}_1 \vec{p}_2 \\ \vec{q}_1 \vec{q}_2}} e^{-i(p_1 - q_1) x_1} e^{-i(p_2 - q_2) x_2} \langle \Psi | \hat{a}^{+}_{\sigma_1}(p_1) \dots \hat{a}_{\sigma_1}(q_1) | \Psi_1 \rangle$$

For $\sigma_1 \neq \sigma_2$, find $(p_1 = q_1, p_2 = q_2)$

$$\left(\frac{n_\Psi}{2}\right)^2 g(\vec{x}_1, \vec{x}_2) = \frac{1}{V^2} \sum_{\vec{p}_1, \vec{p}_2} \langle \Psi | \hat{a}^\dagger_{\vec{p}_2 \sigma_2} \hat{a}_{\vec{p}_2 \sigma_2} \hat{a}^\dagger_{\vec{p}_1 \sigma_1} \hat{a}_{\vec{p}_1 \sigma_1} | \Psi \rangle$$

$$= \frac{1}{V^2} \sum_{p_1, p_2} N_{p_1, \sigma_1} N_{p_2, \sigma_2} = \frac{1}{V^2} N_{\sigma_1} N_{\sigma_2} = \left(\frac{n_\Psi}{2}\right)^2$$

$\hookrightarrow = \frac{N}{2}$ in ground state

$\hookrightarrow$ no effect for $\sigma_1 = \sigma_2$

For $\sigma_1 = \sigma_2 \equiv \sigma$, have either $\vec{p}_1 = \vec{q}_1$ & $\vec{p}_2 = \vec{q}_2$ or $\vec{p}_1 = \vec{q}_2$ & $\vec{p}_2 = \vec{q}_1$

Two contributions:

$$\left(\frac{n_\Psi}{2}\right)^2 g_{\sigma,\sigma}(x_1, x_2) = \left(\frac{n_\Psi}{2}\right)^2 - \left| \frac{1}{V} \sum_{\vec{p}} e^{-i\vec{p}(\vec{x}_1 - \vec{x}_2)} N_{\vec{p}\sigma} \right|^2$$

$$\rightsquigarrow \quad g_{\sigma,\sigma}(\vec{x}_1 - \vec{x}_2) = 1 - 9\left(\frac{\sin\alpha - \alpha\cos\alpha}{\alpha^3}\right)^2 \qquad \alpha = p_F |\vec{x}_1 - \vec{x}_2| .$$

Short distance: $\sin\alpha - \alpha\cos\alpha \approx \frac{1}{3}\alpha^3 \quad (\alpha \ll 1)$

$$\Rightarrow \lim_{|x_1 - x_2| \to 0} g_{\sigma,\sigma}(\vec{x}_1 - \vec{x}_2) = 0$$

$\alpha \gg 1$: $\quad g_{\sigma\sigma}(\vec{x}_1, \vec{x}_2) = 1 \qquad \left(\frac{\sin\alpha}{\alpha} \xrightarrow{\alpha \to \infty} 0\right).$

Opposite of bosonic behavior.

Interpretation: If particle w. spin σ is at x_1, unlikely to find another σ particle nearby!

3.2.2 interacting Fermions

Consider now a ~~system of~~ gas of Electrons, interacting via a Coulomb potential:

$$U^{(2)}(\vec{x}_1 - \vec{x}_2) = \frac{e^2}{|\vec{x}_1 - \vec{x}_2|}$$

Fourier transform: $\tilde{U}^{(2)}(\vec{p}) = \frac{4\pi e^2}{\vec{p}^{\,2}}$

Hamiltonian

$$\hat{H} = \sum_{\vec{p},\sigma} \frac{p^2}{2m} \hat{a}^\dagger_{\vec{p},\sigma} \hat{a}_{\vec{p},\sigma} + \frac{1}{2V} \sum_{\substack{p_1 p_2 q_1 q_2 \\ \sigma_1 \sigma_2 \\ |p_1 - q_1| \neq 0}} \delta_{p_1+p_2,\, q_1+q_2} \times$$

$$\cancel{\times \tilde{U}(\vec{p}_1 - \vec{q}_1)\, \hat{a}^\dagger_1 \hat{a}^\dagger_2 \hat{a}_2 a_1}$$

$$\times \tilde{U}(\vec{p}_1 - \vec{q}_1)\, \hat{a}^\dagger_{\vec{p}_1\sigma_1} \hat{a}^\dagger_{\vec{p}_2\sigma_2} \hat{a}_{q_2\sigma_2} \hat{a}_{q_1\sigma_1}$$

Note: U is divergent for $\vec{p} \to 0$. Infrared singularity
Omitting $|p_1 - q_1| = 0$ in the sum corresponds to choosing a scheme ~~#~~ to regulate the divergence.

↳ QFT 1, 2.

Position space: $\hat{H} = \sum_r \left(-\frac{1}{2m}\Delta_r\right) + \frac{1}{2}\sum_{r\neq s} \hat{U}(\vec{x}_r, \vec{x}_s)$

As usual, we are interested in the ground state.

Hartree - Fock approximation

Assumption

$$|\Psi_0\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(1) & \cdots & \varphi_1(N) \\ \vdots & & \vdots \\ \varphi_N(1) & \cdots & \varphi_N(N) \end{vmatrix}$$

with $\varphi_i(j)$ to be determined.

Let E_0 denote the ground state energy. Have

$$\langle\Psi|\hat{H}|\Psi\rangle \geq E_0 \qquad \text{for arbitrary } |\Psi\rangle .$$

$\Rightarrow$ If we ~~get~~ can guess a good approximation to the ground state, we get an upper bound on E_0.

First, consider $\quad |\Psi\rangle = \prod_{|\vec{p}| \leq p_F} \prod_{\sigma} \hat{a}^{\dagger}_{p,\sigma} |0\rangle .$

Kinetic energy:

$$E_{kin} = \sum_{\vec{p},\sigma} \frac{p^2}{2m} \Theta(p_F - |\vec{p}|)$$

$$= 2 \frac{V}{(2\pi)^3} \int_{|\vec{p}| \leq p_F} d^3p \, \frac{p^2}{2m} = \frac{4\pi V}{(2\pi)^3 m} \int_0^{p_F} dp \, p^4$$

$$E_{kin} = \frac{4\pi V}{(2\pi)^3\, 5m}\, p_F^5 = \frac{3}{5} E_F N .$$

Potential energy:

$$E_{pot} = \frac{4\pi e^2}{2V} \sum_{\substack{p_1 p_2 q_1 q_2 \\ \sigma_1, \sigma_2 \\ |p_1 - q_1| \neq 0}} \frac{\delta_{\vec{p}_1+\vec{p}_2,\, \vec{q}_1+\vec{q}_2}}{(\vec{p}_1-\vec{q}_1)^2} \langle \psi |\, \hat{a}^\dagger_{p_1\sigma_1} \hat{a}^\dagger_{p_2\sigma_2} \hat{a}_{q_2\sigma_2} \hat{a}_{q_1\sigma_1} | \psi \rangle$$

Non-vanishing expt. value only for $\vec{p}_1 = \vec{q}_2$, ~~since~~ $\vec{p}_2 = \vec{q}_1$, $\sigma_1 = \sigma_2$. (Note: Pauli P., only one particle per state).

$$= \frac{4\pi e^2}{2V} \sum_{\vec{p}_1 \neq \vec{p}_2,\, \sigma} \frac{1}{(\vec{p}_1-\vec{p}_2)^2} \langle \psi |\, \hat{a}^\dagger_{p_1\sigma} \hat{a}^\dagger_{p_2\sigma} \hat{a}_{p_1\sigma} \hat{a}_{p_2\sigma} | \psi \rangle$$

$$= -\frac{4\pi e^2}{V} \sum_{p_1 \neq p_2} \frac{1}{(\vec{p}_1-\vec{p}_2)^2} \Theta(p_F - |\vec{p}_1|)\, \Theta(p_F - |\vec{p}_2|)$$

$$= -\frac{4\pi e^2}{V} \frac{V^2}{(2\pi)^6} \int d^3p_1 \int d^3p_2 \frac{\Theta(p_F - |\vec{p}_1|)\, \Theta(p_F - |\vec{p}_2|)}{(\vec{p}_1-\vec{p}_2)^2}$$

Have that
$$\int d^3p_2 \frac{\Theta(p_F - |\vec{p}_2|)}{(\vec{p}_1-\vec{p}_2)^2} = 4\pi\, p_F\, F\!\left(\frac{|\vec{p}_1|}{p_F}\right)$$

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right|$$

$$\Rightarrow E_{pot} = -\frac{e^2 V p_F}{4\pi^4 \hbar} \int_{|\vec{p}_1| < p_F} d^3p_1 \, F\left(\frac{|\vec{p}_1|}{p_F}\right)$$

$$= -\frac{e^2 V p_F^4}{\pi^3} \int_0^1 dx \, x^2 F(x)$$

$$= -\frac{e^2 V}{4\pi^3} p_F^4 = -\frac{3e^2}{4\pi} p_F N .$$

$$E = E_{kin} + E_{pot} = \frac{3}{5} \epsilon_F N - \frac{3e^2 p_F}{4\pi} N .$$

and $E_0 \leq E$.

Now, allow ~~consider~~ variations of $\varphi_i(\vec{x}_j)$ to minimise E .

constraint: $\int |\varphi_i(\vec{x}_j)|^2 d^3x_j = 1$

↳ Lagrange multipliers .

Functional:

$$E(\varphi_1^*, \dots, \varphi_N^*, \varphi_1 \dots \varphi_N) = \langle \Psi | \hat{H} | \Psi \rangle - \sum_{i=1}^{N} E_i \left(\int d^3x \, |\varphi_i(\vec{x})|^2 - 1 \right)$$

where $|\Psi\rangle$ is the usual Slater determinant .

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$$\langle \Psi | \hat{H} | \Psi \rangle = \frac{1}{N!} \int d^3x_1 \dots d^3x_N \begin{vmatrix} \varphi_1^*(\vec{x}_1) & \dots \\ \vdots & \dots \end{vmatrix} \hat{H} \begin{vmatrix} \varphi_1(\vec{x}_1) & \dots & \\ \vdots & \ddots & \varphi_N(\vec{x}_N) \end{vmatrix}$$

$$= \int d^3x_1 \dots d^3x_N \, \varphi_1^*(\vec{x}_1) \dots \varphi_N^*(\vec{x}_N) \, \hat{H} \begin{vmatrix} \varphi_1(\vec{x}_1) & \dots & \varphi_1(\vec{x}_N) \\ \vdots & \ddots & \vdots \\ \varphi_N(\vec{x}_1) & \dots & \varphi_N(\vec{x}_N) \end{vmatrix}$$

$$= \sum_{i=1}^{N} \int d^3x \, \varphi_i^*(x) \left(\frac{-\Delta}{2m} \right) \varphi_i(\vec{x}) \qquad \text{(chain rule)}$$

$$+ \frac{1}{2} \sum_{i \neq j} \int d^3x \int d^3y \, \varphi_i^*(x) \varphi_j^*(y) \, \hat{U}(\vec{x}, \vec{y}) \left(\varphi_i(\vec{x}) \varphi_j(\vec{y}) - \varphi_j(\vec{x}) \varphi_i(\vec{y}) \right)$$

For the lowest energy state, have

$$\frac{\delta E(\varphi_1^* \dots \varphi_N)}{\delta \varphi_i^*(\vec{x})} = 0$$

$$\Rightarrow \quad -\frac{\Delta}{2m} \varphi_i(\vec{x}) + \frac{1}{2} \sum_{i \neq j} \int d^3y \, \varphi_j^*(\vec{y}) \, \hat{U}(\vec{x}, \vec{y}) \left[\varphi_i(\vec{x}) \varphi_j(\vec{y}) - \varphi_j(\vec{x}) \varphi_i(\vec{y}) \right]$$

$$- E_i \varphi_i(\vec{x}) = 0 .$$

Hartree-Fock equations.

Coupled system of N equations for φ_i, $i = 1, \dots, N$, and E_i, $i = 1, \dots, N$.

$\hookrightarrow$ Bad for humans. Good for computers

Molecular Physics / Quantum chemistry

Superconductivity 3.2.3

Observation (1911): At very low temperatures, the electrical resistance of some materials vanishes.

QM explanation, core points:

- In metals, the effective electron-electron interaction is attractive
- The ground state consists of so called Cooper-pairs
- There is a band gap from GS to excited states.

Metal: Atoms sit on lattice sites. Valence electrons delocalised, can move freely. Phonons = lattice oscillations

Coulomb interaction (of electrons):

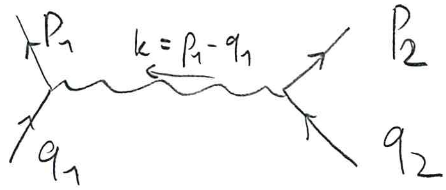
$$\hat{H}_C = \frac{1}{2V} \sum_{\substack{\vec{p}_1 \vec{p}_2 \vec{q}_1 \vec{q}_2 \\ \sigma_1 \sigma_2 \\ \vec{p}_1 - \vec{q}_1 \neq \vec{0}}} \delta_{\vec{p}_1+\vec{p}_2, \vec{q}_1+\vec{q}_2} \tilde{V}_C(\vec{p}_1-\vec{q}_1)\, \hat{a}^\dagger_{\vec{p}_1\sigma_1} \hat{a}^\dagger_{\vec{p}_2\sigma_2} \hat{a}_{\vec{q}_2\sigma_2} \hat{a}_{\vec{q}_1\sigma_1}$$

$$\tilde{V}_C(\vec{p}) = \frac{4\pi e^2}{\vec{p}^2}$$

described by photon exchange.

Electron interaction with phonons (= lattice)
$\Rightarrow$ additional e-e interaction mediated by phonons
(derivation later).

Kinematics



Write $E^e_{\vec p} = \frac{p^2}{2m} - E_F$, (electron energy relative to Fermi energy)

$E^{\text{phonon}}_{\vec p}$ = energy of phonon with momentum $\vec p$.

$g_{\vec q, \vec k}$ = coupling of electron (momentum $\vec q$) with phonon ($\vec k$)

Then the potential due to phonon exchange is given by

$$\hat H_{\text{phonon}} = \frac{1}{2V} \sum_{\substack{p_1 q_1 p_2 q_2 \\ \sigma_1 \sigma_2}} \delta_{p_1+p_2,\, q_1+q_2}\, \tilde V_{\text{phonon}}\, \hat a^+_{p_1\sigma_1} \hat a^+_{p_2\sigma_2} \hat a_{q_2\sigma_2} \hat a_{q_1\sigma_1}$$

with

$$\tilde V_{\text{phonon}} = 2\, g_{\vec q_1 \vec k}\, g_{\vec q_2, -\vec k} \frac{E^{\text{phonon}}_{\vec k}}{\left(E^e_{p_1} - E^e_{q_1}\right)^2 - \left(E^{\text{phonon}}_{\vec k}\right)^2}$$

and $g_{-q,-k} = g^*_{q,k}$.

Obtain

$$\frac{p^2}{m}\tilde{\Psi}(p) + \int \frac{d^3q}{(2\pi)^3}\, \tilde{U}_{eff}(p-q)\,\tilde{\Psi}(q) = (E+2E_F)\,\tilde{\Psi}(\vec{p})$$

Interested in bound states, i.e. solutions with $E<0$. These would lower the energy compared to the states of the free system.

Simplify:
$$U(\vec{p},\vec{q}) = \begin{cases} -\tilde{U}_0 \ , & E_F < \frac{p^2}{2m} < E_F+\Delta E \ ; \ E_F < \frac{q^2}{2m} < E_F+\Delta E \\ 0 & \text{else} \ . \end{cases}$$

$\Rightarrow$

$$\left(\frac{p^2}{m} - E - 2E_F\right)\tilde{\Psi}(p) = \underbrace{\tilde{U}_0 \int \frac{d^3q}{(2\pi)^3}\, \Theta\!\left(\frac{q^2}{2m} - E_F\right)\Theta\!\left(E_F+\Delta E - \frac{q^2}{2m}\right)\tilde{\Psi}(q)}_{\equiv\, C \ (p\text{-independent})}$$

$$\Rightarrow \quad \tilde{\Psi}(p) = \frac{C}{\frac{p^2}{m} - E - E_F}$$

$$\Rightarrow \quad C = \tilde{U}_0 \int \frac{d^3q}{(2\pi)^3}\, \Theta\!\left(\frac{q^2}{2m} - E_F\right)\Theta\!\left(E_F+\Delta E - \frac{q^2}{2m}\right) \frac{C}{\frac{p^2}{2m} - E - E_F}$$

Bound states exist if this equation has a solution with $E<0$.

Integrate:

$$\tilde{U}_0 \int \frac{d^3q}{(2\pi)^3}\, \Theta(\ldots)\, \Theta(\ldots)\, \frac{1}{\frac{q^2}{m} - E - E_F}$$

$$= \tilde{U}_0 \frac{4\pi}{(2\pi)^3} \int q^2 dq\, \Theta\left(\frac{q^2}{2m} - E_F\right) \Theta\left(E_F + \Delta E - \frac{q^2}{2m}\right) \frac{1}{\frac{q^2}{m} - E - 2E_F}$$

$$= \tilde{U}_0 \frac{4\pi}{(2\pi)^3} \sqrt{2}\, m^{3/2} \int_{E_F}^{E_F+\Delta E} dE_q \frac{\sqrt{E_q}}{2E_q - E - 2E_F} \overset{!}{=} 1 .$$

Interested in region with $\Delta E \ll E_F \Rightarrow \sqrt{E_q} \approx \sqrt{E_F}$ and

$$1 = \frac{\sqrt{2}\, m^{3/2}\, \tilde{U}_0 \sqrt{E_F}}{2\pi^2} \ln\left(\frac{2\Delta E - E}{-E}\right)$$

$$= \frac{\rho(E_F)\, \tilde{U}_0}{2} \ln\left(\frac{2\Delta E - E}{-E}\right)$$

where we used $\frac{N}{V} = \frac{2\sqrt{2}\, m^{3/2} E_F^{3/2}}{3\pi^2}$ and $\rho(E_F) \equiv \frac{d}{dE_F}\frac{N}{V}$

Solve for E:

$$E = -2\Delta E \frac{\exp\left(-\frac{2}{\rho(E_F)\tilde{U}_0}\right)}{1 - \exp\left(-\frac{2}{\rho(E_F)\tilde{U}_0}\right)}$$

$$\overset{\rho U \ll 1}{=} -2\Delta E\, e^{-\frac{2}{\rho(E_F)\tilde{U}_0}}$$

$\Rightarrow$ Bound states may exist, even for infinitesimal $\tilde{U}_0$.

This bound state is called <u>Cooper pair</u>.

The solution is symmetric, $\tilde{\Psi}(-p) = \tilde{\Psi}(p)$, i.e. $\Psi(x_1, x_2) = \Psi(x_2, x_1)$.
$\Rightarrow$ spins should be opposite.

generator: $\hat{a}^{+}_{\vec{p}\uparrow} \hat{a}^{+}_{-\vec{p}\downarrow}$

destructor: $\hat{a}_{-\vec{p}\downarrow} \hat{a}_{\vec{p}\uparrow}$

BCS ansatz for ground state:

$$|\Psi_0\rangle = \prod_{\vec{p}} \left(u_{\vec{p}} + v_{\vec{p}} \hat{a}^{+}_{\vec{p},\uparrow} \hat{a}^{+}_{-\vec{p}\downarrow} \right) |0\rangle$$

with $|u_p|^2 + |v_p|^2 = 1$ (normalisation).

Now, consider the effective Hamiltonian

$$\hat{H} = \sum_{p,\sigma} \underbrace{E_p}_{= \frac{p^2}{2m}} \hat{a}^{+}_{p,\sigma} \hat{a}_{p,\sigma} + \underbrace{\frac{1}{V} \sum_{p,q} \tilde{U}_{eff}(p,q) \hat{a}^{+}_{p\uparrow} \hat{a}^{+}_{-p\downarrow} \hat{a}_{-q\downarrow} \hat{a}_{q\uparrow}}_{\text{interaction between Cooper pairs}}$$

We need to further simplify the Hamiltonian.

Mean field approximation

Consider operators $\hat{A}, \hat{B}$ and numbers $\langle \hat{A} \rangle, \langle \hat{B} \rangle$ such that

$$\hat{A} |\Psi_0\rangle \approx \langle \hat{A} \rangle |\Psi_0\rangle$$
$$\hat{B} |\Psi_0\rangle \approx \langle \hat{B} \rangle |\Psi_0\rangle$$

for fixed $|\Psi_0\rangle$. Now consider the product $\hat{A}\hat{B}$:

$$\hat{A}\hat{B} = \left(\langle \hat{A} \rangle + (\hat{A} - \langle \hat{A} \rangle)\right)\left(\langle \hat{B} \rangle + (\hat{B} - \langle \hat{B} \rangle)\right)$$

$$= \langle \hat{A} \rangle \langle \hat{B} \rangle + \langle \hat{A} \rangle (\hat{B} - \langle \hat{B} \rangle) + (\hat{A} - \langle \hat{A} \rangle)\langle \hat{B} \rangle + \underbrace{(\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle)}_{\text{neglect}}$$

$$= \langle \hat{A} \rangle \hat{B} + \langle \hat{B} \rangle \hat{A} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

MFA.

Apply for product of Cooper pair operators:

$$\hat{A} = \sum_p \hat{a}^\dagger_{p\uparrow} \hat{a}^\dagger_{-p\downarrow} \Rightarrow \langle \hat{A} \rangle = \sum_p \langle \Psi_0 | \hat{a}^\dagger_{p\uparrow} \hat{a}^\dagger_{-p\downarrow} | \Psi_0 \rangle = \left(\sum_p u_p^* v_p\right)^*$$

$$\hat{B} = \sum_q \hat{a}_{-q\downarrow} \hat{a}_{q\uparrow} \qquad \langle \hat{B} \rangle = \sum_p u_p^* v_p$$

$$\Rightarrow \hat{H} = \hat{T} + \frac{1}{V} \sum_{pq} \tilde{U}_{\text{eff}}(p,q) (u_p^* v_p)^* \hat{a}_{-q\downarrow} \hat{a}_{q\uparrow}$$

$$+ \frac{1}{V} \sum_{pq} \tilde{U}_{\text{eff}} (u_q^* v_q) \hat{a}^\dagger_{p\uparrow} \hat{a}^\dagger_{-p\uparrow} - \underbrace{\frac{1}{V} \sum_{pq} \tilde{U}_{\text{eff}} (u_p^* v_p)^* (u_q^* v_q)}_{(\equiv \sum \Delta_p u_p v_p^*)}$$

Define the <u>gap-function</u>

$$\Delta_p = -\frac{1}{V}\sum_q \hat{U}_{eff}\, u_q^* v_q$$

$$\Rightarrow \hat{H} = C_0 + \sum_{p,\sigma} \epsilon_p \hat{a}^+_{p\sigma}\hat{a}_{p\sigma} - \sum_p \Delta_p^* \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow} - \sum_p \Delta_p \hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow}$$

Quadratic, but not diagonal. Can try Bogoliubov trafo:

$$\hat{b}_{p,\downarrow} = v_{-p}\hat{a}^+_{-p\uparrow} + u_{-p}\hat{a}_{p\downarrow}$$
$$\hat{b}^+_{p\uparrow} = u_p^* \hat{a}^+_{p\uparrow} - v_p^* \hat{a}_{-p\downarrow}$$

with $|u_p|^2+|v_p|^2=1$.

with the expected anti-commutation relations.

Find
$$\hat{H} = C_0 + \sum_p \left(2\epsilon_p |v_p|^2 + \Delta_p^* u_p^* v_p + \Delta_p u_p v_p^*\right)$$
$$+\sum_p \left[\epsilon_p(|u_p|^2-|v_p|^2) + \Delta_p^* u_p^* v_p + \Delta_p u_p v_p^*\right]\left(\hat{b}^+_{p\uparrow}\hat{b}_{p\uparrow} + \hat{b}^+_{-p\downarrow}\hat{b}_{-p\downarrow}\right)$$
$$+\sum_p \left\{\underbrace{\left[2\epsilon_p u_p v_p - \Delta_p u_p^2 - \Delta_p^* v_p^2\right]}_{=0}\hat{b}^+_{p\uparrow}\hat{b}^+_{-p\downarrow} + \left[\quad\right]^* \hat{b}_{-p\downarrow}\hat{b}_{p\uparrow}\right\}$$

solve for u_p, v_p.

$$\rightsquigarrow \hat{H} = E_0 + \sum_p \sqrt{\epsilon_p^2 + |\Delta_p|^2}\left(\hat{b}^+_{p\uparrow}\hat{b}_{p\uparrow} + \hat{b}^+_{-p\downarrow}\hat{b}_{-p\downarrow}\right)$$

$$E_0 = \sum_p \left(\epsilon_p - \frac{1}{2}\sqrt{\epsilon_p^2 + |\Delta_p|^2}\right)$$

Finally. A diagonal $\hat{H}$. b^+, b create (annihilate) quasi-particles with energies

$$E_p^{quasi} = \sqrt{\mathcal{E}_p^2 + |\Delta_p|^2} \geq |\Delta_p|$$

If $\Delta_p \neq 0$, there is a band gap, at least $|\Delta_p|$ of energy needed to excite a Cooper-pair.

$$\Delta_p = -\frac{1}{V}\sum_q \tilde{U}_{eff}(p,q)\, u_q^* v_q = -\frac{1}{2V}\sum_q \frac{\tilde{U}_{eff}(p,q)\,\Delta_q}{\sqrt{\mathcal{E}_q^2 + |\Delta_q|^2}}$$

$$\approx -\frac{1}{2(2\pi)^3}\int d^3q\, \frac{\tilde{U}_{eff}(p,q)\,\Delta_q}{\sqrt{\mathcal{E}_q^2 + |\Delta_q|^2}}$$

Given $\tilde{U}_{eff}$, can be solved numerically.

For $\tilde{U}_{eff}(p,q) = \begin{cases} -\tilde{U}_0 \,, & 0 < \mathcal{E}_p < \Delta\mathcal{E} \text{ and } 0 < \mathcal{E}_q < \Delta\mathcal{E} \\ 0 \,, & \text{else} \end{cases}$

assume $\Delta_p \equiv \Delta$ constant, and $\Delta \ll \Delta\mathcal{E} \ll E_F$

$$\Delta = \frac{4\sqrt{2}\,\pi\, m^{3/2}\,\tilde{U}_0 \Delta}{2(2\pi)^3}\int_{E_F}^{E_F+\Delta\mathcal{E}} dE \frac{\sqrt{\mathcal{E}}}{\sqrt{(\mathcal{E}-\mathcal{E}_F)^2 + \Delta^2}}$$

$$\approx \frac{2\sqrt{2}}{(2\pi)^3}\, m^{3/2} E_F^{1/2}\,\tilde{U}_0 \Delta \int_0^{\Delta\mathcal{E}} \frac{d\mathcal{E}}{\sqrt{E^2 + \Delta^2}}$$

$$= \frac{1}{4}\,\rho(\mathcal{E}_F)\,\tilde{U}_0\,\Delta \ln\left(2\frac{\Delta\mathcal{E}}{\Delta}\right)$$

$$\Rightarrow \quad \Delta = 2\,\Delta E \, \exp\left(-\frac{4}{\rho(E_F)\,\tilde{V}_0}\right)$$

Now, proceed as with the case of superfluidity.

Current = electrons moving with some velocity

Lab frame: Conductor at rest, e^- moving with $-\vec{v}$. (K)

e^- rest frame: Conductor moving with $\vec{v}$ (K')

As before: $$E = E' - \vec{v}\,\vec{P}' + \frac{1}{2} M \vec{v}^{\,2}$$

$$P = \vec{P}' - M\vec{v} \, .$$

Assume that system K' has e^- in the ground state $|\Psi_0\rangle$.

$$\Rightarrow \quad E_i' = E_0' \qquad \vec{P}_i' = \vec{0} \qquad \text{initial state}$$

and $$E_i = E_0' + \frac{1}{2} M \vec{v}^{\,2} \qquad \vec{P}_i = -M\vec{v}$$

Resistance occurs due to scatterings with atoms etc.
$\Leftrightarrow$ excitation of quasiparticles in system K'.

Consider excitation of one quasi-particle of momentum $\vec{p}'$

$$\Rightarrow \quad E_f' = E_0' + E^{quasi}_{\vec{p}'} \qquad \vec{P}_f' = \vec{p}'$$

and $\quad E_f = E_0' + E^{quasi}_{\vec{p}'} - \vec{v}\vec{p}' + \frac{1}{2}M\vec{v}^2 \qquad \vec{P}_f = \vec{p}' - M\vec{v}$

$$\Rightarrow \quad \Delta E = E_f - E_i = E^{quasi}_{\vec{p}'} - \vec{v}\vec{p}'$$

and $\Delta E < 0$ for a process where the electrons loose kinetic energy, i.e. electric resistance. Not possible if

$$|\vec{v}| < \frac{E^{quasi}_{\vec{p}}}{|\vec{p}'|} = \frac{1}{|\vec{p}'|}\sqrt{\left(\frac{p'^2}{2m} - E_F\right)^2 + |\Delta_{\vec{p}'}|^2}$$

For sufficiently small velocities, the current flows without resistance.

Prediction of BCS theory:

$$\Delta_p = -\frac{1}{V}\sum_q \tilde{U}_{eff}\, u_q^* v_q$$

$$= -\frac{1}{V}\sum_q \tilde{U}_{eff}\langle \hat{a}_{-q\downarrow}\hat{a}_{q\uparrow}\rangle$$

$$= -\frac{1}{V}\sum_q \tilde{U}_{eff}\, u_q^* v_q \left(1 - 2\hat{b}^+_{q\uparrow}\hat{b}_{q\uparrow}\right)$$

$$= -\frac{1}{V}\sum_q \tilde{U}_{eff}\, u_q^* v_q \left(1 - 2n_F\left(E_q^{quasi}\right)\right) \qquad n_F(E) = \frac{1}{e^{\beta E}+1}$$

Fermi-Dirac distribution

$$\Rightarrow \quad \Delta = \frac{1}{4}\,\rho(E_F)\,\tilde{U}_0 \int_0^{\Delta E} dE\, \frac{\Delta}{2\sqrt{E^2+\Delta^2}} \left(1 - 2n_F\left(\sqrt{E^2+\Delta^2}\right)\right)$$

$$\Leftrightarrow \quad \frac{2}{\tilde{U}_0\,\rho(E_F)} = \int_0^{\Delta E} dE\, \frac{1}{\sqrt{E^2+\Delta^2}} \tanh\left(\beta\sqrt{E^2+\Delta^2}/2\right)$$

Solve for $T=0 \Leftrightarrow \beta=\infty$, $\Delta_0 = 2\Delta E \exp\left(-\frac{4}{\rho(E_F)\,\tilde{U}_0}\right)$

Solve for T_c, given by $\Delta = 0$.

$$T_c \approx 1.13\,\Delta E \exp\left(-\frac{4}{\rho(E_F)\,\tilde{U}_0}\right)$$

$$\Rightarrow \quad \frac{2\Delta_0}{T_c} \approx 3.5$$ agrees well with data.

Symmetry argument: $\rightarrow$ QFT.

Note: High T_c superconductors still poorly understood.

Scattering processes (3.3)

The cross section

Usual situation:

Expect that the number of scattering events is proportional to ρ_A, ρ_B, l_A, l_B and transverse overlap F.

Define cross section σ.

$$\underset{\substack{\uparrow \\ \text{intrinsic} \\ \text{property of particles A,B}}}{\sigma} = \frac{\#\,\text{scattering events}}{\underbrace{\rho_A\, l_A\, \rho_B\, l_B\, F}_{\text{macroscopic quantities}}}$$

differential cross section

$$\frac{d\sigma}{d^3p_1 \cdots d^3p_N}$$ with N particles with momenta $p_1, \dots, p_N$ in final state

Reason: Often detectors don't cover full angle

The S-matrix (3.3.2)

Formal (mathematical) description of scattering process:

2 incoming, n outgoing particles, well separated at $t = -\infty$ and $t = +\infty$.

$\Rightarrow$ Describe initial and final states as products of free single particle wave functions.

For proper normalisation: Use wave packets

$$|\phi\rangle = \int \frac{d^3k}{(2\pi)^3} \phi(\vec{k}) |\vec{k}\rangle$$

with $\phi(\vec{k})$ peaking at $\vec{p}$. Furthermore $\langle \vec{q}|\vec{p}\rangle = \delta^3(\vec{p}-\vec{q})$ and

$$\langle \phi|\phi\rangle = \int \frac{d^3k}{(2\pi)^3} \frac{|\phi(\vec{k})|^2}{(2\pi)^3} \stackrel{!}{=} 1$$

Initial state ($t = -\infty$)

$$|\phi_A \phi_B\rangle_{in} = \int \frac{d^3k_A}{(2\pi)^3} \int \frac{d^3k_B}{(2\pi)^3} \phi_A(\vec{k}_A)\, \phi_B(\vec{k}_B)\, e^{-i\vec{b}\vec{k}_B} |\vec{k}_A \vec{k}_B\rangle_{in}$$

transverse displacement of wave packets

$|\vec{b}|$ is ~~often~~ called impact parameter!

For the final state, use ${}_{out}\langle \vec{p}_1 \vec{p}_2 \cdots \vec{p}_N |$.

For an arbitrary time dependent Hamiltonian, have

$$|\psi, t\rangle = T \exp\left\{-i \int_{t_0}^{t} dt' \hat{H}\right\} |\psi, t_0\rangle,$$

Here T is the time ordering operater:

$$T(\hat{A}(t_1)\hat{B}(t_2)) = \hat{A}(t_1)\hat{B}(t_2)\,\Theta(t_1 - t_2) + \hat{B}(t_2)\hat{A}(t_1)\,\Theta(t_2 - t_1)$$

[for bosons].

To calculate ${}_{out}\langle \vec{p}_1 \cdots \vec{p}_N | \vec{k}_A, \vec{k}_B \rangle_{in}$, use

$${}_{out}\langle \vec{p}_1 \cdots \vec{p}_N | \vec{k}_A \vec{k}_B \rangle_{in}$$

$$= \langle \vec{p}_1 \cdots \vec{p}_N | T \exp\left(-i \int_{-\infty}^{+\infty} dt\, \hat{H}\right) | \vec{k}_A \vec{k}_B \rangle$$

We define the $\hat{S}$ operater as

$$\hat{S} = T \exp\left(-i \int_{-\infty}^{+\infty} dt\, \hat{H}\right)$$

The S-matrix are the matrix elements of $\hat{S}$:

$$\langle \vec{p}_1 \cdots \vec{p}_N | \hat{S} | \vec{k}_A \vec{k}_B \rangle = {}_{out}\langle \vec{p}_1 \cdots \vec{p}_N | \vec{k}_A \vec{k}_B \rangle_{in}$$

If the particles don't interact, then $\hat{S} = \mathbb{1}$. Useful to extract the nontrivial part in general:

$$\hat{S} \equiv \mathbb{1} + i (2\pi)^4 \, \delta^4\Big(k_A + k_B - \sum_f p_f\Big) \hat{T}$$

4-vectors

Energy-momentum conservation

transition operator

The matrix elements of $\hat{T}$ are called (transition) amplitudes

$$i\mathcal{A}(k_A k_B \to p_1 \cdots p_N) \equiv \langle \vec{p}_1 \cdots \vec{p}_N | i\hat{T} | \vec{k}_A \vec{k}_B \rangle$$

Given initial states A,B, interested in the probability to observe certain final states:

$$P = \Big(\prod_f \int d^3 p_f \Big) \left| {}_{out}\langle \vec{p}_1 \cdots \vec{p}_N | \phi_A \phi_B \rangle_{in} \right|^2$$

To get the cross section, integrate over $\vec{b}$.

$$\sigma = \int d^2 p \; P(\vec{b}) \, .$$

For the differential cross section, we now find

$$\frac{d\sigma}{d^3p_1 \ldots d^3p_N} = \int d^2 p \left(\prod_{i=A,B} \int \frac{d^3k_i}{(2\pi)^3} \phi_i(\vec{k}_i) \int \frac{d^3k_i'}{(2\pi)^3} \phi_i^*(\vec{k}_i') \right) \times$$

$$\times \; e^{-i\vec{b}(\vec{k}_B - \vec{k}_B')} \; {}_{out}\langle \vec{p}_1 \ldots \vec{p}_N | \vec{k}_A \vec{k}_B \rangle_{in} \; {}_{out}\langle \vec{p}_1 \ldots \vec{p}_N | \vec{k}_A' \vec{k}_B' \rangle_{in}^*$$

We are not interested in the trivial ($\hat{S} - \hat{1}$) part, therefore can use

$${}_{out}\langle \vec{p}_1 \ldots \vec{p}_N | \vec{k}_A \vec{k}_B \rangle_{in} = (2\pi)^4 \delta^4\Big(k_A + k_B - \sum_f p_f \Big) \, i\mathcal{A}(k_A k_B \to p_1 \ldots p_N)$$

and same for k_A', k_B'.

We can use $\delta^4(k_A' + k_B' - \sum_f p_f)$ and the $\delta^2(k_B^\perp - k_B'^\perp)$ from integrating $e^{i\vec{b}(\vec{k}_B - \vec{k}_B')}$ over transverse directions, to perform all k' integrals.

$$\int \frac{d^3k_A'}{(2\pi)^3} \int \frac{d^3k_B'}{(2\pi)^3} (2\pi)^2 \delta^2(k_B^\perp - k_B'^\perp) \, (2\pi)^4 \delta^4(k_A' + k_B' - k_A - k_B)$$

$$=$$

$$= \int dk_A^{z'} \int dk_B^{z'} \, \delta(E_A' + E_B' - E_A - E_B) \, \delta(k_A^{z'} + k_B^{z'} - k_A^z - k_B^z)$$

$$= \int dk_A^{z'} \, \delta(E_A' + E_B' - E_A - E_B) \Big|_{k_B^{z'} = k_A^z + k_B^z - k_A^{z'}}$$

Now, remember that $\delta(g(x)) = \dfrac{\delta(x - x_0)}{|g'(x_0)|}$ where $g(x_0) = 0$

$$= \frac{1}{\left| \frac{\partial E_A'}{\partial k_A^{z'}} - \frac{\partial E_B'}{\partial k_B^{z'}} \right|} = \frac{1}{|v_A - v_B|}$$

relative velocity in laboratory frame.

Intermediate result:

$$\frac{d\sigma}{dp_1 \ldots} = \int \frac{d^3k_A}{(2\pi)^3} \frac{d^3k_B}{(2\pi)^3} |\phi_A(\vec{k}_A)|^2 |\phi_B(\vec{k}_B)|^2 (2\pi)^4 \delta^4(k_A + k_B - \sum_f p_f) \times$$
$$\times \frac{1}{|v_A - v_B|} |A(k_A k_B \to p_1 \ldots p_N)|^2$$

Now, detectors can only determine momenta with finite precision. Since $\phi_{A,B}$ are peaked at $\vec{p}_A, \vec{p}_B$, can replace $k_{A,B} \to p_{A,B}$ in terms that depend continuously on $k_{A/B}$. Furthermore we can replace $\delta(k_A + k_B \to \sum_f p_f)$ with $\delta(p_A + p_B - \sum_f p_f)$

Find

$$\frac{d\sigma}{d^3p_1 \dots d^3p_N} = (2\pi)^6 \frac{1}{|v_A - v_B|} |A(p_A p_B \rightarrow p_1 \dots p_N)|^2 (2\pi)^4 \delta^4(p_A + p_B - \sum_f p_f)$$

↳ See also Peskin Schröder, sec. 4.5.

Causality (3.3.3)

Consider $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$

$\hat{H}_0$: free theory; $\hat{H}_1$: interactions

Assume that $\hat{H}_0$ is time independent, and that the solutions are known:

$$\hat{H}_0 |\psi_n^0\rangle = E_{n,0} |\psi_n^0\rangle .$$

↳ n runs over free many particle states + their quantum numbers

Schrödinger equ. for interacting theory:

$$i \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$

$$\Leftrightarrow \left(i \frac{\partial}{\partial t} - \hat{H}_0 \right) |\psi\rangle = \lambda \hat{H}_1 |\psi\rangle$$

Now search for Green's function of differential operator on LHS:

$$\left(i\frac{\partial}{\partial t} - \hat{H}_0\right)\hat{G}_0(t,t') = \mathbb{1}\cdot\delta(t-t')$$

$\mathbb{1} = \delta^3(\vec{x}-\vec{x}')$ for 1-particle states

Note: $\hat{G}_0$ is an operator → Green's operator.

Using $\hat{G}_0$ we obtain an integral equ. for $|\psi,t\rangle$

$$|\psi,t\rangle = |\psi^0,t\rangle + \lambda\int_{-\infty}^{+\infty} dt'\,\hat{G}_0(t,t')\,\hat{H}_1(t')\,|\psi,t'\rangle$$

Check:

$$\left(i\frac{\partial}{\partial t} - \hat{H}_0\right)|\psi,t\rangle = \left(i\frac{\partial}{\partial t} - \hat{H}_0\right)|\psi^0,t\rangle + \lambda\int_{-\infty}^{+\infty} dt'\,\delta(t-t')\,\hat{H}_1(t')\,|\psi,t'\rangle$$

$$= \lambda\,\hat{H}_1(t)\,|\psi,t\rangle$$

Since $\hat{H}_0$ is assumed to be time independent, we find two Greens functions:

$$\hat{G}_0^+(t,t') = -i\,\Theta(t-t')\,e^{-i\hat{H}_0(t-t')}$$ retarded Green's operator

$$\hat{G}_0^-(t,t') = i\,\Theta(t'-t)\,e^{-i\hat{H}_0(t-t')}$$ advanced Green's operator

Consider the case where $\hat{H}_1$ is "switched on" at $t = t_0$. Causality implies that $|\psi, t\rangle$ should be affected by $\hat{H}_1$ only for $t > t_0$.

Guaranteed by using retarded GO:

$$|\psi, t\rangle = |\psi^0, t\rangle + \lambda \int_{-\infty}^{+\infty} dt' \, G_0^+(t,t') \, \hat{H}_1(t') \, |\psi, t'\rangle$$

$\sim \Theta(t - t^0) \Rightarrow$ causality.

Can write $\hat{G}_0^+(t,t') = \hat{G}_0^+(t-t')$. Fourier transform:

$$\hat{G}_0^+(t) = \int \frac{dE}{2\pi} \, e^{-iEt} \, \hat{\tilde{G}}_0(E)$$

with $E \to E + i\delta$ and $\delta > 0$. [$t > 0$ for retarded GO, s.th. $e^{-i(i\delta)t} = e^{\delta t}$. Close contour below to get finite result for $t > 0$ case, picking up potential poles at $\mathrm{Im}(E) = 0$.]

Inverse FT:

$$\hat{\tilde{G}}_0^+(E) = \int_{-\infty}^{+\infty} dt \, e^{i(E+i\delta)t} \, \hat{G}_0^+(t) = -i \int_0^{\infty} dt \, e^{i(E+i\delta - \hat{H}_0)t}$$

$$= \frac{1}{E + i\delta - \hat{H}_0} \qquad \text{"resolvent"}$$

Here $e^{-i\delta t}$ ensures that the integral vanishes at $+\infty$.

Now, consider for a moment the case where also $\hat{H}_1(t)$ is time independent. Then

$$|\psi,t\rangle = e^{-iEt}|\psi\rangle \quad \text{, and we must solve } \hat{H}|\psi\rangle = E|\psi\rangle$$

$$\Leftrightarrow \qquad (E-\hat{H}_0)|\psi\rangle = \lambda \hat{H}_1|\psi\rangle$$

$$\Rightarrow \qquad |\psi\rangle = |\psi_0\rangle + \lambda \frac{1}{E+i\delta-\hat{H}_0}\hat{H}_1|\psi\rangle$$

Lippmann - Schwinger equ.

Iterative solution :

$$|\psi\rangle = |\psi_0\rangle + \lambda (E+i\delta-\hat{H}_0)^{-1}\hat{H}_1|\psi_0\rangle$$
$$+ \lambda^2 (E+i\delta-\hat{H}_0)^{-1}\hat{H}_1 (E+i\delta-\hat{H}_0)^{-1}\hat{H}_1|\psi^0\rangle + \mathcal{O}(\lambda^3)$$

$\boxtimes$

Time dependent case :

$$|\psi,t\rangle = |\psi_0,t\rangle + \lambda\int_{-\infty}^{+\infty} dt_1\, \hat{G}_0^+(t,t_1)\,\hat{H}_1(t_1)\,|\psi^0,t_1\rangle$$
$$+ \lambda^2 \int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{+\infty} dt_2\, \hat{G}_0^+(t,t_1)\,\hat{H}_1(t_1)\,\hat{G}_0^+(t_1,t_2)\,\hat{H}_1(t_2)\,|\psi,t_2\rangle + \mathcal{O}(\lambda^3)$$

$$= |\psi^0, t\rangle - i\lambda \int_{-\infty}^{t} dt_1\, e^{-i\hat{H}_0(t-t_1)} \hat{H}_1(t_1) |\psi^0, t_1\rangle$$

$$- \lambda^2 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2\, e^{-i\hat{H}_0(t-t_1)} \hat{H}_1(t_1) e^{-i\hat{H}_0(t_1-t_2)} \hat{H}_1(t_2) |\psi^0, t_2\rangle + \mathcal{O}(\lambda^3)$$

Perturbation theory (3.3.4)

Goal: Find S-matrix elements for given $\hat{H}_1$, as perturbative series in λ.

Interaction picture:

Define $\hat{U}_0 = T \exp\left(-i \int_{t_0}^{t} dt_1\, \hat{H}_0\right) = \exp^{-i\hat{H}_0(t-t_0)}$

and

$$|\psi, t\rangle_I = \hat{U}_0(t)^\dagger |\psi, t\rangle$$

$$(\hat{H}_1)_I(t) = \hat{U}_0(t)^\dagger \hat{H}_1(t) \hat{U}_0(t)$$

$$\Rightarrow \quad i\frac{\partial}{\partial t} |\psi, t\rangle_I = \lambda (\hat{H}_1)_I(t) |\psi, t\rangle_I$$

Solution: $|\psi, t\rangle_I = T \exp\left(-i\lambda \int_{t_0}^{t} dt_1 (\hat{H}_1)_I(t_1)\right) |\psi, t_0\rangle_I$

Expand for small λ:

$$|\psi,t\rangle_I = |\psi,t_0\rangle_I - i\lambda\int_{t_0}^{t} dt_1 (\hat{H}_1)_I(t_1)\,|\psi,t_0\rangle_I$$

$$- \lambda^2 \int_{t_0}^{t} dt_1\,(\hat{H}_1)_I(t_1)\int_{t_0}^{t_1} dt_2\,(\hat{H}_1)_I(t_2)\,|\psi,t_0\rangle_I + \mathcal{O}(\lambda^3)$$

Now, connect with S. Let the system be in $|\psi_i^0\rangle$ at t_i. Interested in probability to find state $|\psi_f^0\rangle$ at time t_f, where $|\psi^0\rangle$ are the eigenstates of $\hat{H}_0$.

$$\Rightarrow \quad S_{fi} = {}_I\langle \psi_f^0 |\, T\exp\left(-i\lambda\int_{t_i}^{t_f} dt_1 (\hat{H}_1)_I(t_1)\right) | \psi_i^0\rangle_I$$

Use that

$$(\hat{H}_1)_I(t_1) = \exp(i\hat{H}_0(t_1-t_i))\,\hat{H}_1(t_1)\exp(-i\hat{H}_0(t_1-t_i))$$

$$= \sum_{j,k} \exp(i\hat{H}_0(t_1-t_i))|\psi_j^0\rangle\underbrace{\langle\psi_j^0|\hat{H}_1(t_1)|\psi_k^0\rangle}_{M_{jk}}\langle\psi_k^0|\exp(-i\hat{H}_0(t_1-t_i))$$

$$= \sum_{j,k} e^{iE_{j,0}(t_1-t_i)}\,|\psi_j^0\rangle\, M_{jk}\,\langle\psi_k^0|\,e^{-iE_{k,0}(t_1-t_i)}$$

and $\quad |\psi_f^0\rangle_I = e^{iE_{f,0}(t_f-t_i)}\,|\psi_f^0\rangle$

$$\Longrightarrow S_{fi} = e^{-iE_{f,0}(t_f-t_i)} \times$$

$$\times \langle \psi_f^0 | T \exp\Big(-i\lambda \sum_{jk} \int_{t_i}^{t_f} dt_1\, e^{-i(E_{k,0}-E_{j,0})(t_1-t_i)} |\psi_j^0\rangle M_{jk} \langle \psi_k^0|\Big) | \psi_i^0 \rangle$$

We can expand $S_{fi} = \sum_{l=0}^{\infty} \lambda^l S_{fi}^{(l)}$

$$S_{fi}^{(l)} = (-i)^l \sum_{j_1 j_2 \cdots j_{l-1}} \int_{t_i}^{t_f} dt_l \int_{t_i}^{t_l} dt_{l-1} \cdots \int_{t_i}^{t_2} dt_1 \times$$

$$\times e^{-iE_f^0(t_f-t_l)} M_{f j_{l-1}} e^{-iE^0_{j_{l-1}}(t_l-t_{l-1})} M_{j_{l-1} j_{l-2}} \cdots e^{iE^0_{j_1}(t_2-t_1)} M_{j_1 i} e^{-iE_i^0(t_1-t_i)}$$

Very abstract. Should consider an <u>example:</u> System with electrons and phonons:

$$\hat{H} = \underbrace{\sum_{\vec{p},\sigma} E_{\vec{p}}^e \hat{a}^+_{\vec{p}\sigma} \hat{a}_{\vec{p}\sigma}}_{\text{electrons}} + \underbrace{\sum_{\vec{p}} E_{\vec{p}}^\gamma \hat{b}^+_{\vec{p}} b_{\vec{p}}}_{\text{phonons}} \qquad (= \hat{H}_0)$$

$$+ \frac{1}{\sqrt{V}} \sum_{\vec{p}\vec{k}\vec{q},\sigma} g_{\vec{q},\vec{k}}\, \delta_{\vec{p},\vec{q}+\vec{k}}\, \hat{a}^+_{\vec{p},\sigma} \hat{a}_{\vec{q},\sigma} (\hat{b}^+_{-\vec{k}} + \hat{b}_{\vec{k}}) \qquad (= \hat{H}_1)$$

NR system: $\epsilon_{\vec{p}}^e = \frac{\vec{p}^2}{2m}$, $\epsilon_{\vec{p}}^\gamma = v_\gamma |\vec{p}|$, $v_\gamma \ll c\ (=1)$.

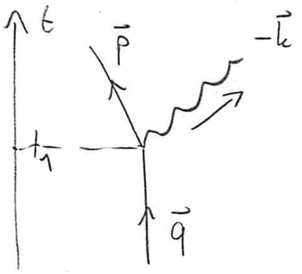
Now, consider a process $e^-(\vec{q}\uparrow) \longrightarrow e^-(\vec{p}\uparrow) + \gamma(-\vec{k})$

$$\Rightarrow \quad |i\rangle = \hat{a}^+_{\vec{q}} |0\rangle \qquad |f\rangle = \hat{a}^+_{\vec{p}} \hat{b}^+_{-\vec{k}} |0\rangle$$

(drop spin. Not changed in interaction)

$$E_i = E^{e}_{\vec{q}} \,, \quad E_f = \epsilon^{e}_{\vec{p}} + E^{\gamma}_{-\vec{k}} \;.$$

Picture (Feynman diagram):



Note: We do not know t_1, that is why it is integrated over

$$S^{(1)}_{fi} = -i \int_{t_i}^{t_f} dt_1 \exp\left(-i E_f (t_f - t_1)\right) \langle f | \hat{H} | i \rangle \exp\left(-i E_i (t_1 - t_i)\right)$$

$$= -i \exp\left(-i (E_f t_f - E_i t_i)\right) \int_{t_i}^{t_f} dt_1 \, e^{i(E_f - E_i) t_1} \langle f | \hat{H}_1 | i \rangle$$

Calculate the matrix element:

$$\langle f | \hat{H}_1 | i \rangle = \frac{1}{\sqrt{V}} \langle 0 | \hat{b}_{-k} \hat{a}_p \Big(\sum_{p'k'q'} g_{q'k'} \delta_{p', q'+k'} \hat{a}^{+}_{p'} \hat{a}_{q'} (\hat{b}^{+}_{k'} + \hat{b}_{-k'}) \Big) \hat{a}^{+}_q | 0 \rangle$$

$$= \frac{1}{\sqrt{V}} g_{qk} \delta_{p, q+k}$$

With $t_{f,i} \to \pm \infty$, find

$$S_{fi} = -\frac{i}{\sqrt{V}} g_{qk} \delta_{p,q+k} e^{-i(E_f t_f - E_i t_i)} \int_{-\infty}^{+\infty} dt_1 \, e^{-i(E_f - E_i) t_1}$$

$$= -\frac{2\pi i}{\sqrt{V}} e^{-i E_i (t_f - t_i)} g_{q,k} \delta_{p,q+k} \delta(E_f - E_i)$$

drops out of probability, due to $| \; |^2$.

momentum conservation

energy conservation