LECTURE 9

Electrons in the presence of MANY IMPURITIES:

Theory of electrical resistance in metals.

- We will see that in the presence of many random impurities electrons acquire finite life time.

$$G(\vec{p},t) \rightarrow -i\theta(t)\, e^{-i\varepsilon_p t - \Gamma_p t} \qquad \Gamma_p > 0$$

Read Sec. 5.1 from textbook for a discussion of how this irreversible behavior emerges from a perfectly unitary evolution in a quantum system.

One-electron GF in a many-impurity system

$$H = \frac{p^2}{2m} + \sum_i U(\vec{x} - \vec{X}_i) \qquad \vec{X}_i \text{ - random impurity positions}$$

Second Q:

$$\boxed{H = \sum_p \varepsilon_p c_p^+ c_p + \sum_q U(\vec{q})\, \rho_q \sum_p c_{p+q}^+ c_p}$$

$$\sum_i U(\vec{x} - \vec{X}_i) = \sum_i \sum_q e^{i\vec{q}(\vec{x}-\vec{X}_i)}\, U(\vec{q})$$

$$= \sum_q e^{i\vec{q}\vec{x}}\, U(\vec{q}) \underbrace{\sum_i e^{-i\vec{q}\cdot\vec{X}_i}}_{\rho_q}$$

The eq. of motion is $\quad (T=0)$

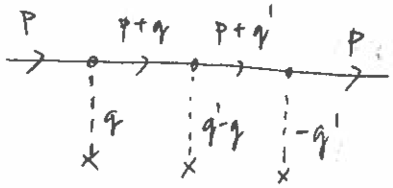
$$\left(i\frac{\partial}{\partial t} - \varepsilon_p\right) F(p,p';t) = \delta_{pp'}\,\delta(t) + \sum_q U(q)\rho_q\, F(p+q,p';t)$$

- we pass to frequency representation and solve by iteration:

$$F(p,p') = G^0(p)\Big[\delta_{pp'} + U(p-p')\rho_{p-p'}\,G^0(p') + \sum_q U(q)\rho_q\,G^0(p+q)\,U(p-q-p')\rho_{p-q-p'}\,G^0(p') + \dots\Big]$$

For one-electron GF $\quad G(p) \equiv F(p,p)$

$$G(p) = G^0(p) + G^0(p)\left[U(q)\rho_q\right]_{q=0} G^0(p) + G^0(p)\Big[\sum_q U(q)\rho_q\,G^0(p+q)\,U(-q)\rho_{-q}\Big]G^0(p) +$$

$+$  $+ \;\dots$

Averaging over impurity positions

We are interested in AVERAGED GF

$$\overline{G}(p) = \int \left(\prod_{i=1}^{N} \frac{1}{V} d^3 x_i \right) G[\vec{x}_1, \dots \vec{x}_N]$$

$\vec{x}_i$ only enter in $\rho_q = \sum_i e^{-i\vec{q}\cdot\vec{x}_i}$ so we need to average products of ρ_q's:

1st order:

$$\overline{\rho_q} = \frac{N}{V} \int d^3 x \, e^{-i\vec{q}\cdot\vec{x}} = N \delta_{q0}$$

2nd order:

$$\overline{\rho_{q_1} \rho_{q_2}} = \sum_{i \neq j} \overline{e^{-i\vec{q}_1\cdot\vec{x}_i} e^{-i\vec{q}_2\cdot\vec{x}_j}} + \sum_i \overline{e^{-i(\vec{q}_1+\vec{q}_2)\cdot\vec{x}_i}}$$

$$= N^2 \delta_{q_1 0} \delta_{q_2 0} + N \delta_{q_1+q_2, 0}$$

$$\rightarrow \overline{\rho_q \rho_{-q}} = N^2 \delta_{q,0} + N$$

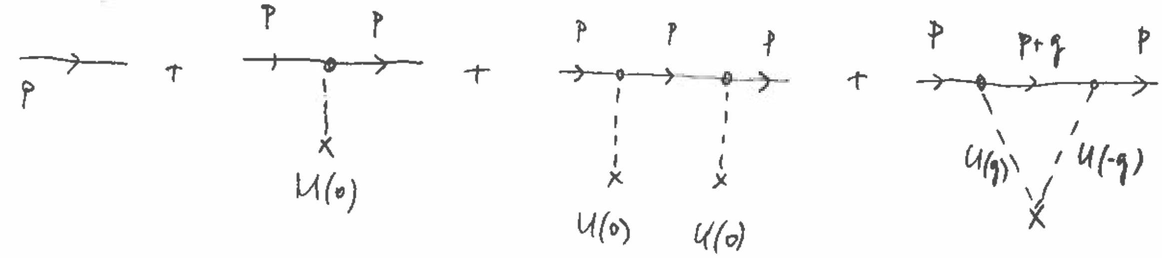
$$\overline{G}(p) = G^0(p) + G^0(p) \left[U(q) \overline{\rho_q} \right]_{q=0} G^0(p)$$

$$+ G^0(p) \left[\sum_q U(q) G^0(p+q) U(-q) \overline{\rho_q \rho_{-q}} \right] G^0(p) + \dots$$

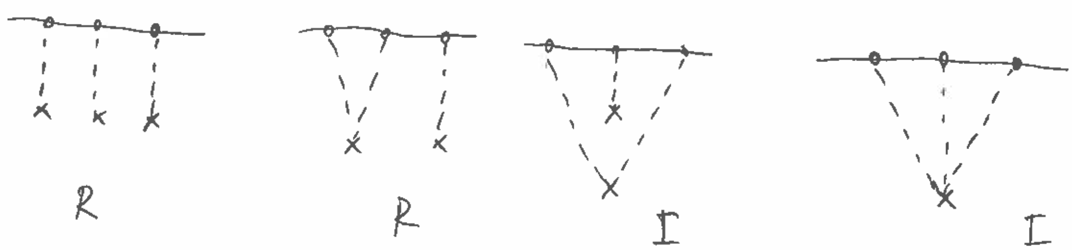
$$= G^0(p) + G^0(p) \left[U(0) N \right] G^0(p)$$

$$+ G^0(p) \left[N^2 U(0) G^0(p) U(0) + N \sum_q U(q) G^0(p+q) U(-q) \right] G^0(p)$$

$$+ \dots$$

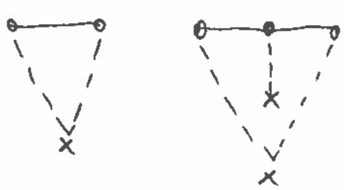
$\bar{G}(p) =$ 

3rd order



Irreducible diagrams and Dyson's equation

- Irreducible diagram cannot be divided into sub-diagrams by cutting one fermion line
- Irreducible self-energy diagram is an irreducible diagram with the $G^0(p)$ lines removed on both ends:



$$+ \dots = \sum_{i=1}^{\infty} \Sigma^{(i)}(\vec{p}, \varepsilon) \equiv \Sigma(\vec{p}, \varepsilon)$$

total irreducible self-energy

The exact GF can be written in terms of the exact self energy as

$$G(p) = G^0(p) + G^0(p)\,\Sigma(p,\varepsilon)\,G^0(p) + $$
$$+ G^0(p)\,\Sigma(p,\varepsilon)\,G^0(p)\,\Sigma(p,\varepsilon)\,G^0(p) + \dots$$

$$= G_0(p) + G^0(p)\,\Sigma(p,\varepsilon)\left[G^0(p) + G^0(p)\,\Sigma(p,\varepsilon)\,G^0(p) + \dots\right]$$

$$= G_0(p) + G^0(p)\,\Sigma(p,\varepsilon)\,G(p)$$

$$\Rightarrow \boxed{G(p) = \frac{1}{[G^0(p)]^{-1} - \Sigma(p,\varepsilon)} = \frac{1}{\varepsilon - \varepsilon_p - \Sigma(p,\varepsilon)}}$$

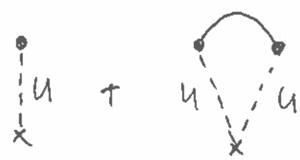
Dyson's equation

- We can now focus on calculating the self-energy. $\Sigma(p,\varepsilon)$.
- Including a single diagram in $\Sigma(p,\varepsilon)$ amounts to summing up an infinite series in the expansion of $G(p)$

Low-density, weak scattering approximation

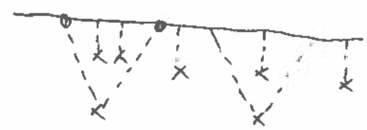
- low density of impurities: N/V is small

- weak scattering: $U(\vec{x})$ is small

$\Sigma(\vec{p}, \varepsilon) \simeq$ 

N/V $\qquad$ N/V

← first order in N/V, second order in U

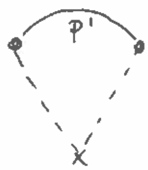


"second order Born approximation"

$n_{imp} = \frac{N}{V}$

- first order  $= N\, U(0) = n_{imp} \int d^3x\, U(\vec{x})$

absorb into electron energy
$\varepsilon_p \to \varepsilon_p + N U(0)$

- second order 

$$= N \sum_{p'} U(p-p')\, G^0(p')\, U(p'-p)$$

$$= N \sum_{p'} U^2(p-p')\, G^0(p')$$

Assume
Short range potential $\quad U(\vec{x}) = U\,\delta(\vec{x}) \;\Rightarrow\; U(\vec{p}) = \frac{U}{V}$

$$\Sigma(\varepsilon) = n_{imp} \frac{U^2}{V} \sum_{p'} G^0(p') \xrightarrow[N/V = \text{const}]{V \to \infty} n_{imp}\, U^2 \int d^3p'\, G^0(p')$$

$$\Sigma(\varepsilon) = n_{imp} U^2 \int d^3p \, \frac{1}{\varepsilon - \varepsilon_p + i\eta}$$

$$= n_{imp} U^2 \int d\varepsilon' \, \frac{\rho(\varepsilon')}{\varepsilon - \varepsilon' + i\eta}$$

$$\rho(\varepsilon') = \int d^3p \, \delta(\varepsilon' - \varepsilon_p)$$

↑ density of electron states

$$\frac{1}{x + i\eta} = \mathcal{P}\frac{1}{x} - i\pi\delta(x)$$

$$\Sigma(\varepsilon) = n_{imp} U^2 \left[\int d\varepsilon' \mathcal{P}\left(\frac{\rho(\varepsilon')}{\varepsilon - \varepsilon'}\right) - i\pi\delta(\varepsilon) \right]$$

further shift in energy ε_p

Δ

finite life time

$-i\Gamma$

$$\boxed{G(\vec{p};\varepsilon) = \frac{1}{\varepsilon - \varepsilon_p - \Delta + i\Gamma}}$$

If for a moment we treat Δ and Γ as ε-indep. constants then

$$G(\vec{p},t) = \int_{-\infty}^{\infty} d\varepsilon \, e^{-i\varepsilon t} G(\vec{p},\varepsilon) = \int_{-\infty}^{\infty} d\varepsilon \, \frac{e^{-i\varepsilon t}}{\varepsilon - \varepsilon_p - \Delta + i\Gamma}$$

$$= -i \, e^{-i(\varepsilon_p + \Delta)t} \, e^{-t\Gamma}$$

electron decay rate

→ irreversible behavior