Lecture 3.

Transport theories of metals and semiconductors (cont.)

- Formalism of Green functions and Feynman diagrams
- Kubo formula for conductivity
- Charge and spin currents
- Spin Hall effect

Calculation of current (quantum mechanics)

Current operator:

$$\hat{j}_i = \frac{e\hbar K_i}{m} = -\frac{ie\hbar}{m}\nabla_i$$

$\vec{K}$ is wave vector

QM average:

$$j_i = \sum_n \int d^3r\, \psi_n^*(\vec{r})\, \hat{j}_i\, \psi_n(\vec{r}) =$$

Sum over occupied states

$$= -\frac{ie\hbar}{m}\sum_n \int d^3r\, \psi_n^*(\vec{r})\, \nabla_i\, \psi_n(\vec{r})$$

$\psi_n(r)$ is the solution of Schödinger equation

$$\hat{\mathcal{H}}\,\psi_n(\vec{r}) = \varepsilon_n \psi_n(\vec{r})$$

and $\hat{\mathcal{H}}$ is the Hamiltonian

$$\hat{\mathcal{H}} = \frac{\hbar^2\hat{K}^2}{2m} + \underbrace{V(\vec{r})}_{\text{impurities}} = -\frac{\hbar^2}{2m}\nabla_i^2 + V(\vec{r})$$

We also need electric field!

Electromagnetic field in Hamiltonian:

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\left(\nabla_i - \frac{ie}{\hbar c}A_i\right)^2 + e\varphi + V(\vec{r})$$

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \nabla\varphi$$

We take the gauge with $\varphi = 0$ and $\vec{A} = \vec{A}(t)$, i.e. $\vec{E}$ is homogeneous

Generalization:

$$\vec{E}(t) = \vec{E}_0 e^{-i\omega t}$$

$$\Rightarrow \quad \vec{A}(t) = \vec{A}_0 e^{-i\omega t}$$

$$\boxed{\vec{A}_0 = \frac{c}{i\omega}\vec{E}_0}$$

Suppose $\vec{A}(t)$ is small (linear response)

$$\hat{\mathcal{H}} = \underbrace{-\frac{\hbar^2}{2m}\nabla_i^2}_{\mathcal{H}_0} + \underbrace{\frac{ie\hbar A_i(t)}{c}\nabla_i + V(\vec{r})}_{W(\vec{r},t)\text{ - small perturbation}}$$

Back to current

$$j_i(t) = -\frac{ie\hbar}{m}\sum_{\substack{n \\ \text{(occupied)}}} \Psi_n^*(\vec{r},t)\left(\nabla_i - \frac{ie}{\hbar c}A_i\right)\Psi_n(\vec{r},t)$$

Free electron:

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{\mathcal{H}}_0\right)\Psi_k(\vec{r},t) = 0$$

Solution: $$\Psi_k(\vec{r},t) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}} e^{-\frac{i\varepsilon_k t}{\hbar}}$$

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

With these $\Psi_k(\vec{r},t)$ we get $j_i = 0$

<u>Trick with perturbation $\hat{W}$</u>

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{\mathcal{H}}_0\right)\Psi(\vec{r}t) = \hat{W}(\vec{r}t)\Psi(\vec{r}t)$$

We introduce Green function:

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{\mathcal{H}}_0\right)G(\vec{r}t,\vec{r}'t') = \delta(\vec{r}-\vec{r}')\,\delta(t-t')$$

$$\Rightarrow \quad \Psi(\vec{r}t) = \Psi_0(\vec{r}t) + \int d^3r'dt'\, G_0(\vec{r}t,\vec{r}'t')\,\hat{W}(\vec{r}'t')\,\Psi(\vec{r}'t')$$

<u>Shorthand</u>: $$x \equiv (\vec{r}t)$$
$$\int dx \equiv \int d^3r\, dt$$

$$\Psi(x) = \Psi_0(x) + \int dx'\, G_0(xx')\,W(x')\,\Psi(x')$$

Series expansion:

$$\psi(x) = \psi_0 + \int dx'\, G_0(xx')\, W(x')\, \psi_0(x') +$$
$$+ \int dx'\, dx_1\, G_0(xx_1)\, W(x_1)\, G_0(x_1 x')\, W(x')\, \psi_0(x') + \ldots$$

Define: $G(xx') = G_0(xx') + \int dx_1\, G_0(xx_1) W(x_1) G_0(x_1 x') + \ldots$

$$\Rightarrow \quad \psi(x) = \psi_0(x) + \int dx_1\, G(xx_1)\, W(x_1)\, \psi_0(x_1)$$

Feynman diagrams

$= G_0(xx')$

$= G(xx')$

$W(x)$

Equation:

We find $G_0(xx')$

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla_i^2\right) G_0(\vec{r}t, \vec{r}'t') = \delta(\vec{r}-\vec{r}')\,\delta(t-t')$$

Homogeneity in space and time:

$$G_0(rt, r't') = \sum_{\varepsilon \vec{k}} G_0(\varepsilon \vec{k})\, e^{i\vec{k}(\vec{r}-\vec{r}')}\, e^{-\frac{i\varepsilon(t-t')}{\hbar}}$$

Fourier transform

$$\sum_{k\varepsilon} = \int \frac{d^3k}{(2\pi)^3}\frac{d\varepsilon}{2\pi}$$

$$\Rightarrow \quad \left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) G_0(\varepsilon \vec{k}) = 1$$

To avoid singularity: $\varepsilon \to \varepsilon + i\delta\, \mathrm{sign}(\varepsilon - \mu)$
(casual GF)

$$\boxed{G_0(\varepsilon \vec{k}) = \frac{1}{\varepsilon - \varepsilon_k + i\delta\, \mathrm{sign}(\varepsilon-\mu)}}$$

Back to the current

$\delta \to +0$

$$j_i(t) = e \sum_{\substack{n \\ \text{(occupied)}}} \int d^3r\, \hat{v}_i\, \Psi_n(\vec{r}t)\, \Psi_n^*(\vec{r}', t+\delta)\Big|_{\vec{r}=\vec{r}'}$$

If there is no field

$$j_i(t) = 2e \sum_{\substack{k \\ \text{(occupied)}}} v_i\, \Psi_k(\vec{r}t)\, \Psi_k^*(\vec{r}', t+\delta)\Big|_{\vec{r}=\vec{r}'} =$$

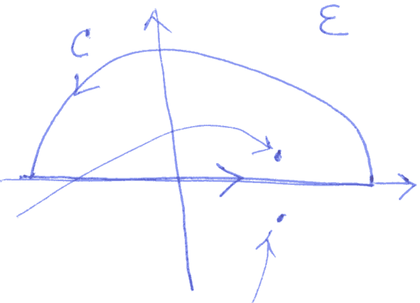
$$= -2ie \sum_{k\varepsilon} v_i\, G_0(\vec{k}, \varepsilon)\, e^{i\varepsilon\delta/\hbar}$$

Indeed:

$$-i\sum_{\varepsilon k} G_0(\varepsilon \vec{k}) = -i\sum_k \int \frac{d\varepsilon}{2\pi} \frac{e^{i\varepsilon\delta}}{\varepsilon - \varepsilon_k + i\delta\, \mathrm{sign}(\varepsilon-\mu)}$$

Poles in ε-plane:

$$\varepsilon = \varepsilon_k - i\delta\, \mathrm{sign}(\varepsilon_k - \mu)$$



If $\varepsilon_k < \mu$, poles in upper half plane

If $\varepsilon_k > \mu$, poles are in lower half plane

$$\Rightarrow -i \sum_{\varepsilon K} G_0(\varepsilon \vec{K}) = \sum_{K<K_F} \cdots$$

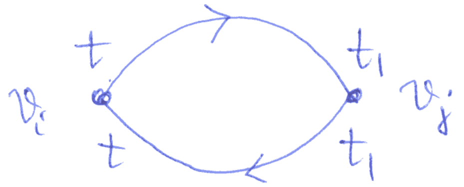
Linear response

$$j_i(t) = -2ie \sum_K v_i G_0(\vec{K}, tt)$$
old formula

$$j_i(t) = -2ie \sum_K v_i\, G(\vec{K}, tt)$$

Only second order in $W(\tau t) = -\frac{e v_i A_i(t)}{c}$

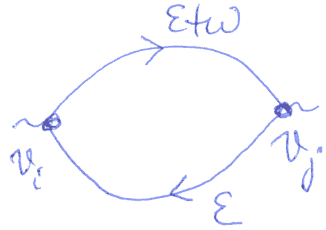
$$\Rightarrow j_i(t) = \frac{2ie^2}{c} \sum_K \int dt_1\, v_i G_0(\vec{K}, tt_1)\, v_j A_j(t_1)\, G_0(\vec{K}, t_1 t)$$



Fourier over t:

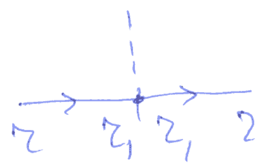
$$\Rightarrow \vec{j} = \vec{j}_0\, e^{-i\omega t}, \qquad j_{0i} = \sigma_{ij} E_{0j}$$

$$\sigma_{ij} = \frac{2e^2}{\omega} \int \frac{d^3k}{(2\pi)^3} \frac{d\varepsilon}{2\pi}\, v_i\, G_0(\vec{k}, \varepsilon+\omega)\, v_j\, G_0(\vec{k}, \varepsilon)$$



But we forgot about impurities!

$$V(\vec{r}) \Rightarrow \sum_i V_i(\vec{r} - \vec{R}_i)$$



We generelize the previous formula:

$$\boxed{\sigma_{ij} = \frac{2e^2}{\omega} \mathrm{Tr} \int \frac{d\varepsilon}{2\pi} \langle v_i\, G(\varepsilon+\omega)\, v_j\, G(\varepsilon) \rangle}$$

Kubo

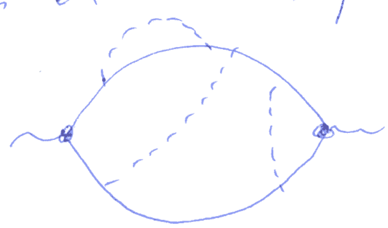
$\langle \ldots \rangle$ average over impurities

Has anybody calculated it with impurities?

Answer: no

Main problem: localization (Anderson)

In Born approximation only second order of interaction on one impurity is accounted



etc.

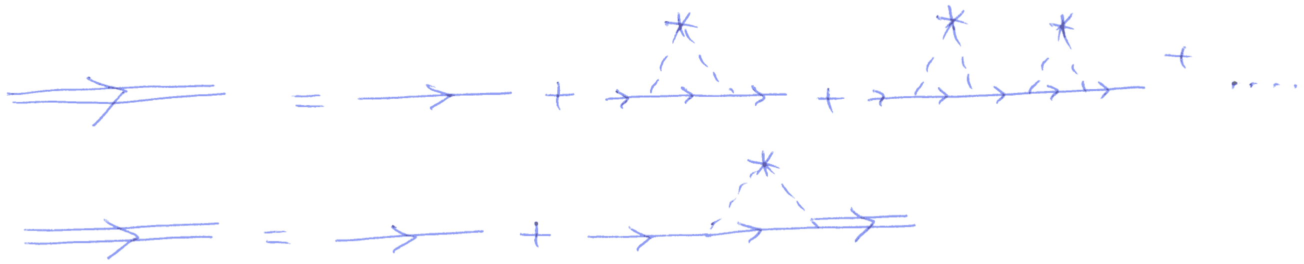
<u>We simplify the problem:</u>

1) only conductivity σ_{ii}

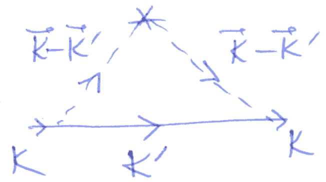
2) impurities in Born approximation

3) short-range impurity potential

Green function should be corrected:



$$G(\vec{k}\,\varepsilon) = G_0(\vec{k}\,\varepsilon) + G_0(\vec{k}\,\varepsilon)\Sigma(\vec{k}\,\varepsilon)G(\vec{k}\,\varepsilon)$$

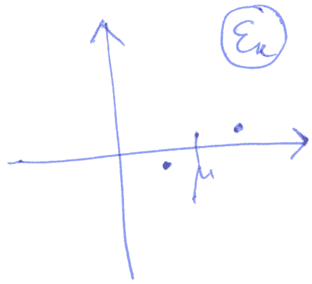
where $\Sigma(\vec{k}\,\varepsilon) =$ 

$$\Sigma(\vec{k}\,\varepsilon) = \int \frac{d^3k'}{(2\pi)^3} \frac{V_{kk'}V_{k'k}}{\varepsilon - \varepsilon_{k'} + i\delta\,\mathrm{sign}(\varepsilon-\mu)} \rightarrow$$

$$\rightarrow V_0^2 \int \frac{d^3k'}{(2\pi)^3} \frac{1}{\varepsilon - \varepsilon_{k'} + i\delta\,\mathrm{sign}(\varepsilon-\mu)}$$

$$\Sigma(\varepsilon) = -\frac{V_0^2}{2} \int \frac{\nu(\varepsilon_k)\,d\varepsilon_k}{\varepsilon_k - \varepsilon - i\delta\,\mathrm{sign}(\varepsilon-\mu)}$$

Pole: $\varepsilon_k = \varepsilon + i\delta\,\mathrm{sign}(\varepsilon-\mu)$



$$\Sigma(\varepsilon) \simeq -i\pi\nu V_0^2 \,\mathrm{sign}(\varepsilon-\mu)$$

We neglect $\mathrm{Re}\,\Sigma$

Define: $\frac{1}{2\tau} = \pi\nu V_0^2$

$$\Rightarrow \quad \Sigma(\varepsilon) = -\frac{i\,\mathrm{sign}(\varepsilon-\mu)}{2\tau}$$

Back to Green function:

$G = G_0 + G_0 \Sigma G$ (Dyson eq.)

$G_0^{-1} = G^{-1} + \Sigma$

$G^{-1} = G_0^{-1} - \Sigma$

$$G_0 = \frac{1}{\varepsilon - \varepsilon_k + i\delta\,\mathrm{sign}(\varepsilon-\mu)}$$

$$\boxed{G(\varepsilon\vec{k}) = \frac{1}{\varepsilon - \varepsilon_k + \frac{i}{2\tau}\mathrm{sign}(\varepsilon-\mu)}}$$

Sciencexpress Research Article

Observation of the Spin Hall Effect in Semiconductors

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