

Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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Today's class: *Kubo formula for conductivity.*

- Current operator.
- Conductivity tensor.
- Linear response: Current-current correlation function.
- Conductance

Current operator

Hamiltonian in equilibrium:
$$H_0 = \frac{1}{2m} \sum_{\sigma} \int d\vec{r} \hat{\psi}_{\sigma}^{\dagger}(\vec{r}) \left(\frac{\hbar}{i} \nabla_r + e\hat{A}(\vec{r}) \right)^2 \hat{\psi}_{\sigma}(\vec{r})$$

In terms of the *current density*:
$$\hat{H}_0 = \hat{K} + e\vec{A} \cdot \left(\mathbf{J}^{\nabla} + \frac{\mathbf{J}^A}{2} \right)$$



$$\left\{ \begin{array}{l} \mathbf{J}^{\nabla} = \frac{i\hbar}{2m} \sum_{\sigma} [(\nabla \psi_{\sigma}^{\dagger}(\vec{r})) \psi_{\sigma}(\vec{r}) - \psi_{\sigma}^{\dagger}(\vec{r}) (\nabla \psi_{\sigma}(\vec{r}))] \text{ “paramagnetic”} \\ \mathbf{J}^A = \frac{e}{m} \vec{A}(\vec{r}) \sum_{\sigma} \psi_{\sigma}^{\dagger}(\vec{r}) \psi_{\sigma}(\vec{r}) = \frac{e}{m} \vec{A}(\vec{r}) \rho(\vec{r}) \text{ “diamagnetic”} \end{array} \right.$$

Perturbation:
$$\vec{A} \rightarrow \vec{A} + \delta\vec{A} \Rightarrow \hat{H} = \hat{H}_0 + \delta\hat{H}$$

$$\delta\hat{H} = e \int d\vec{r} \mathbf{J}_0(\vec{r}) \cdot \delta\vec{A}(\vec{r}) \quad \mathbf{J}_0 = \mathbf{J}^{\nabla} + \mathbf{J}^A$$

Conductivity and linear response

Perturbation “turned on” at t_0 : $\delta\mathbf{E}(\vec{r}, t) = -\frac{\partial}{\partial t}\delta\vec{A}(\vec{r}, t)$

Current density: $\mathbf{J}(\vec{r}, t) = \mathbf{J}_0(\vec{r}, t) + \frac{e}{m}\rho(\vec{r})\delta\vec{A}$

Conductivity tensor: $-e\langle\mathbf{J}(\vec{r}, t)\rangle = \int d\vec{r}' dt' \boldsymbol{\sigma}(\vec{r}, \vec{r}', t') \cdot \delta\mathbf{E}(\vec{r}', t')$

Let's focus on a single component: (say, x)

$$\left\{ \begin{array}{l} -e\langle J(\vec{r}, t)\rangle = \int d\vec{r}' dt' \sigma_{xx}(\vec{r}, \vec{r}', t')\delta E(\vec{r}', t') \\ J(\vec{r}, t) = J_0(\vec{r}, t) + \frac{e}{m}\rho(\vec{r})\delta A \\ \delta E(\vec{r}, t) = -\frac{\partial}{\partial t}\delta A(\vec{r}, t) \Rightarrow \delta E(\vec{r}, \omega) = i\omega\delta A(\vec{r}, \omega) \end{array} \right.$$

Kubo formula for the conductivity

Linear response: $\langle J(\vec{r}, t) \rangle = \langle J(\vec{r}, t) \rangle_0 - i \int_{t_0}^{\infty} dt' \theta(t - t_0) \left\langle \left[J(\vec{r}, t), \delta \hat{H}(t') \right]_- \right\rangle_0$

Perturbation: $\delta \hat{H} = e \int d\vec{r} J_0(\vec{r}, t) \delta A(\vec{r}, t)$ with $\langle J_0(\vec{r}, t) \rangle_0 = 0$
Equilibrium

Kubo formula for the conductivity:

■ $\sigma_{xx}(\vec{r}, \vec{r}', \omega) = \frac{ie^2}{m\omega} \langle \rho(\vec{r}) \rangle_0 \delta(\vec{r} - \vec{r}') + \frac{ie^2}{\omega} \chi_{J_0 J_0}^R(\vec{r}, \vec{r}', \omega)$

with

$\chi_{J_0 J_0}^R(\vec{r}, \vec{r}', \omega) = \langle \langle J_0(\vec{r}) : J_0(\vec{r}') \rangle \rangle_{\omega}$ Current-current correlation function

Conductance

Electric current:

$$\left\{ \begin{array}{l} \vec{J}_e(\vec{r}, t) = -e\vec{J}(\vec{r}, t) \\ I = \int_A dA \vec{n}_\perp \cdot \vec{J}_e(\vec{r} \in A, t) \end{array} \right.$$

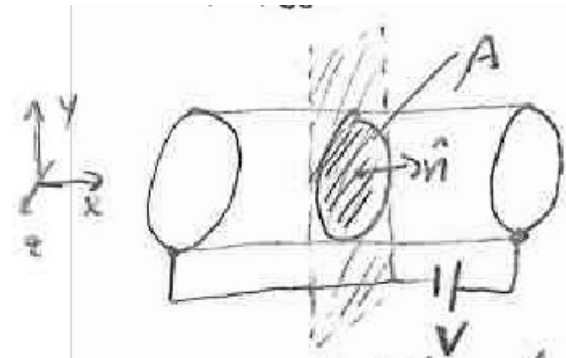
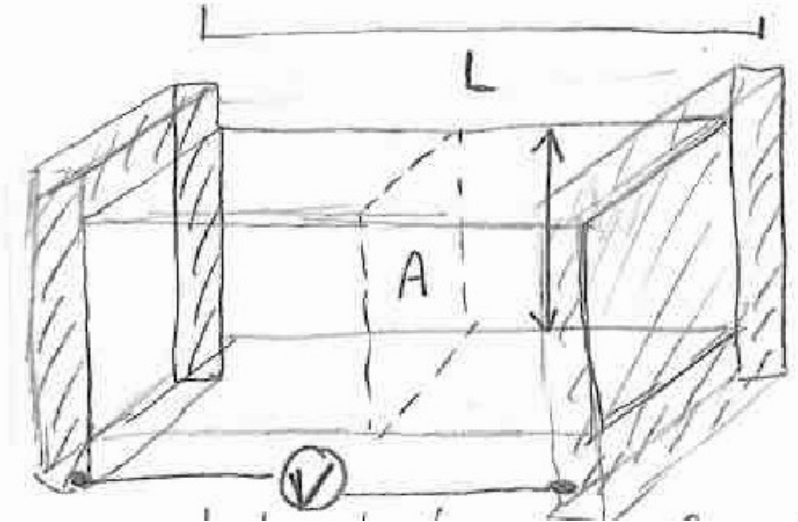
Uniform sample

$$G = \frac{I}{V} = \frac{A}{L} \sigma_{xx}(\omega = 0)$$

dc conductivity

Non-uniform samples

$$I(x) = \int_{A_x} dA \vec{n}_\perp \cdot \vec{J}_e(\vec{r} \in A_x)$$



Conductance

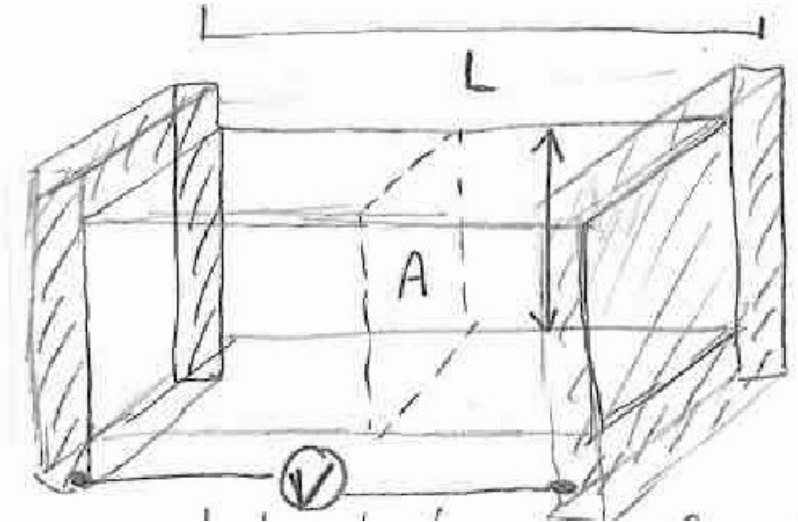
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Uniform sample

$$G = \frac{I}{V} = \frac{A}{L} \sigma_{xx}(\omega = 0)$$

dc conductivity



Non-uniform samples

$$I = \int_A dA \vec{n}_\perp \cdot \vec{J}$$

$$I(x) = \int_0^L G(x, x') E_x(x') dx'$$

■ $G(x, x') = \lim_{\omega \rightarrow 0} \text{Re} \frac{e}{i\omega} \chi_{II}^R(x, x', \omega) E_x(x') dx'$