LECTURE 10

Linear response: Theory of electrical conductivity

- Consider a system of electrons (i.e. metal + impurities) in weak applied electric field $\vec{E}$. Want to find current response to LINEAR ORDER in $\vec{E}$.

$$H_{tot} = \underset{\substack{\uparrow \\ \text{metal}}}{H} + \underset{\substack{\uparrow \\ \text{coupling to } \vec{E}}}{H_{ext}}$$

$$H_{ext} = \int d^3x \, \vec{A}(\vec{x},t) \cdot \vec{j}(x)$$

$\vec{A}(\vec{x},t)$ – vector potential

$\vec{E}(\vec{x},t) = + \frac{\partial}{\partial t}\vec{A}(\vec{x},t) - \vec{\nabla}\phi$

$\vec{j}(x)$: "paramagnetic" component of the total current operator $\vec{J}(\vec{x},t)$

$$\vec{J}(\vec{x},t) = \frac{1}{2}\sum_i \left\{ [\vec{p}_i - e\vec{A}(\vec{x}_i,t)]\,\delta(\vec{x}-\vec{x}_i) + \delta(\vec{x}-\vec{x}_i)\,[\vec{p}_i - e\vec{A}(\vec{x},t)] \right\}$$

$$= \underbrace{\frac{1}{2}\sum_i \left[\vec{p}_i\,\delta(\vec{x}-\vec{x}_i) + \delta(\vec{x}-\vec{x}_i)\,\vec{p}_i \right]}_{\vec{j}(\vec{x})}, - ne\vec{A}(\vec{x},t)$$

Where does this come from?

$$H_0 = \frac{p^2}{2m}$$

Minimal substitution:

$$\vec{p} \to \vec{p} - e\vec{A}$$

$$H_0 \to \frac{1}{2m}(\vec{p} - e\vec{A})^2 = \frac{1}{2m}\Big(\vec{p}^{\,2} \underbrace{- e\vec{p}\cdot\vec{A} - e\vec{A}\cdot\vec{p}}_{\substack{\text{1st order} \\ \text{coupling } H_{ext}}} + \underbrace{e^2\vec{A}^2}_{\substack{\text{2nd order} \\ \text{in } \vec{E}}}\Big)$$

Second quantized current operator

$$\vec{j}(\,) = \sum_{kk'} \langle \vec{k} | \hat{j} | \vec{k}' \rangle c_k^\dagger c_k \qquad |\vec{k}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{x}}$$

$$\boxed{= \sum_{p,p} e^{i\vec{q}\cdot\vec{x}} (\vec{p} + \tfrac{1}{2}\vec{q})\, a_{p+q}^\dagger a_p} \qquad \text{(Check!)}$$

- ## Linear response machinery

Start from the system in an eigenstate $|E_N\rangle$ of H with energy E_N. Turn on $\vec{E}$:

$$i\frac{\partial}{\partial t}|E_N(t)\rangle = H_{tot}|E_N(t)\rangle$$

We can formally solve this by

$$|E_N(t)\rangle = e^{-iHt}\, U_{ext}(t)\, |E_n\rangle$$

$$U_{ext}(t) = 1 - i \int_0^t H_{ext}(t')\, U_{ext}(t')\, dt' \qquad (\text{Check!})$$

Calculate the exp. value of the current density:

$$\langle \vec{J}(\vec{x},t)\rangle_N = \langle E_N(t)|\, \vec{j}(\vec{x})\, |E_N(t)\rangle - ne\vec{A}(\vec{x},t)$$

$$U_{ext}(t) \simeq 1 - i \underbrace{\int_0^t H_{ext}(t')\, dt'}_{I} + \dots \qquad (\text{to lin order in } \vec{A})$$

$$\langle \vec{J}(\vec{x},t)\rangle_N \simeq \langle E_N|\, (1+iI)\, \overset{e^{iHt}}{\vee}\, \vec{j}(\vec{x})\, \overset{e^{-iHt}}{\vee}\, (1-iI)\, |E_N\rangle - ne\vec{A}(\vec{x},t)$$

$$\simeq \langle \vec{j}(\vec{x})\rangle_N + i \langle E_N|\, I\, \vec{j}(\vec{x},t) - \vec{j}(\vec{x},t)\, I\, |E_N\rangle - ne\vec{A}$$

$$= \langle \vec{j}(\vec{x})\rangle_N + i \int_0^t dt' \langle E_n|\, [H_{ext}(t'), \vec{j}(\vec{x},t)]\, |E_N\rangle - ne\vec{A}$$

$$H_{ext}(t) = e^{iHt}\, H_{ext}\, e^{-iHt}, \qquad \vec{j}(\vec{x},t) = e^{iHt}\, \vec{j}(\vec{x})\, e^{-iHt}$$

Kubo formula for linear response.

$$\langle J_\alpha(\vec{x},t)\rangle = \langle j_\alpha(x)\rangle + \int_{-\infty}^{\infty} dt' \int d^3x \; R_{\alpha\beta}(\vec{x}-\vec{x}', t-t')\, \underline{A_\beta(\vec{x}',t')}$$

$$R_{\alpha\beta}(\vec{x}-\vec{x}', t-t') = \mathcal{R}_{\alpha\beta}(\vec{x}-\vec{x}', t-t') - ne\,\delta_{\alpha\beta}\,\delta(\vec{x}-\vec{x}')\,\delta(t-t')$$

$$\mathcal{R}_{\alpha\beta}(\vec{x}-\vec{x}', t-t') = -i\,\theta(t-t')\langle [j_\alpha(\vec{x},t), j_\beta(\vec{x}',t')]\rangle$$

"Retarded current-current correlator"
-evaluated at ZERO FIELD!

- This can be extended to non-zero T situations: by replacing

$$\langle \quad \rangle \rightarrow \langle \quad \rangle_\beta = \frac{1}{Z}\,\mathrm{Tr}\left\{e^{-\beta H}[\hat{j}_\alpha(\vec{x},t), j_\beta(\vec{x},t)]\right\}$$

Evaluation of the Kubo formula for the many-impurity problem

$$j_\alpha(\vec{x}) = \sum_{p,q} e^{i\vec{q}\cdot\vec{x}}\,(\vec{p}+\tfrac{1}{2}\vec{q})\, c^\dagger_{p+q} c_p$$

$\langle [j_\alpha(\vec{x},t), j_\beta(\vec{x}',t')]\rangle$ - involves products of 4 operators

$\rightarrow$ "two-particle Green's function"

Strategy: We will evaluate TIME-ORDERED correlators

$$\mathcal{R}^T_{\alpha\beta}(\vec{x}-\vec{x}', t-t') = -i\langle T[\, j_\alpha(\vec{x},t)\, j_\beta(\vec{x}',t')]\rangle$$

using Wick's theorem and then relate them to corresponding RETARDED correlators via spectral representation (see Eqs. A.2.14-16 textbook).

$$\mathrm{Re}\, \mathcal{R}_{\alpha\beta}(\vec{x},\omega) = \mathrm{Re}\, \mathcal{R}^T_{\alpha\beta}(\vec{x},\omega)$$

$$\mathrm{Im}\, \mathcal{R}_{\alpha\beta}(\vec{x},\omega) = \underline{\mathrm{sgn}(\omega)}\, \mathrm{Im}\, \mathcal{R}^T_{\alpha\beta}(\vec{x},\omega)$$

$$\mathcal{R}^T_{\alpha\beta}(\vec{x}-\vec{x}', t-t') = -i\sum_{p,q}\sum_{p',q'} e^{i\vec{q}\cdot\vec{x}+i\vec{q}'\cdot\vec{x}'} (\vec{p}+\tfrac{1}{2}\vec{q})_\alpha\, (\vec{p}'+\tfrac{1}{2}\vec{q}')_\beta$$

$$\langle T[\, c^+_{p+q}(t)\, c_p(t)\, c^+_{p'+q'}(t')\, c_{p'}(t')]\rangle$$

Fourier transform and use Wick's theorem

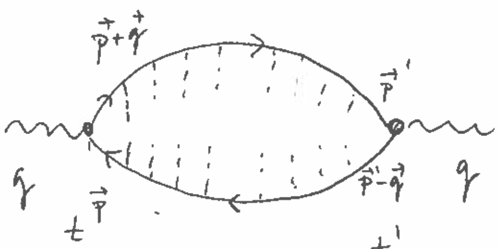
$$\mathcal{R}^T_{\alpha\beta}(\vec{q}, t-t') = -i\sum_{pp'} (p+\tfrac{1}{2}q)_\alpha\, (p'-\tfrac{1}{2}q)_\beta$$

$$F(p, p'-q;\, t-t')\, F(p', p+q;\, t'-t)$$

FT in time and average over impurities:

$$\overline{R^T_{\alpha\beta}(\vec{q},\omega)} = -\frac{i}{2\pi}\int_{-\infty}^{\infty} d\varepsilon \sum_{pp'} \left(p+\tfrac{1}{2}q\right)_\alpha \left(p'-\tfrac{1}{2}q\right)_\beta$$

$$\times\ \overline{F(p,p'-q;\varepsilon+\omega)\,F(p';p+q;\varepsilon)}$$

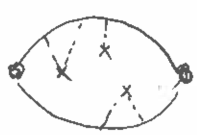
photon 

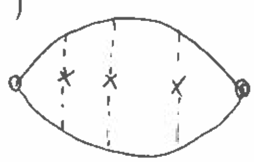
photon

"electron-hole bubble"

before averaging

- Upon averaging over imp. positions we'll encounter diagrams like these

(i) 

(ii) 

(i) - easily taken into account by using averaged one-particle GF obtained previously $\overline{G}(p)$.

(ii) - "vertex corrections"  important to obtain correct transport properties.

- will be included using a "ladder approximation"